



Contents

Preface to the Proceedings of ICM 2002 1725

Papers

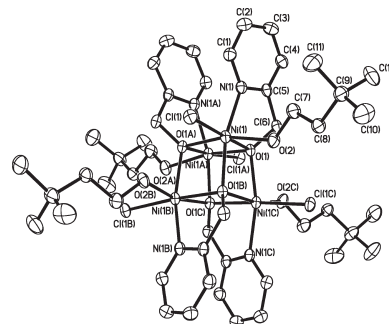
En-Che Yang, Wolfgang Wernsdorfer, Stephen Hill, Rachel S. Edwards, Motohiro Nakano, S. Maccagnano, Lev N. Zakharov, Arnold L. Rheingold, George Christou, David N. Hendrickson

Polyhedron 22 (2003) 1727

Exchange bias in Ni₄ single-molecule magnets

Three Ni₄ cubane single-molecule magnets (SMMs) with composition [Ni(hmp)(ROH)Cl]₄ have been prepared, where R is CH₃ (complex **1**), CH₂CH₃ (complex **2**)

or CH₂CH₂C(CH₃)₃ (complex **3**), and hmp is the anion of 2-hydroxymethylpyridine. All three complexes have been characterized by magnetization measurements and single crystal high-frequency EPR spectra. There are ferromagnetic exchange interactions that give a *S* = 4 ground state with negative magnetoanisotropy. Magnetization versus magnetic field measurements made on single crystals with a micro-SQUID magnetometer indicate these Ni₄ complexes are SMMs. Exchange bias is seen in the magnetization hysteresis loops for complexes **1** and **2**.

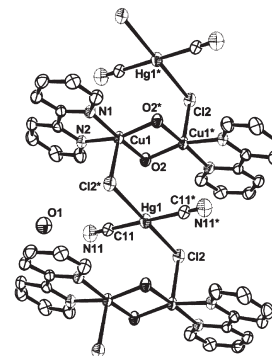


Daniel B. Leznoff, Neil D. Draper, Raymond J. Batchelor

Polyhedron 22 (2003) 1735

Using HgX₂ units (X = Cl, CN) to increase structural and magnetic dimensionality in conjunction with (2,2'-bipyridyl)copper(II) building blocks

Some of the first coordination polymers that incorporate linear, neutral Hg(CN)₂ building blocks have been prepared, as well as a related complex using HgCl₂. These d¹⁰ centers increase structural dimensionality by acting as low-coordinate Lewis acids which accept halide ligands from complex cations in a bridging fashion. The mercury(II) centers mediate weak magnetic exchange between copper(II) ions, thereby increasing the magnetic dimensionality of the coordination polymers as well.

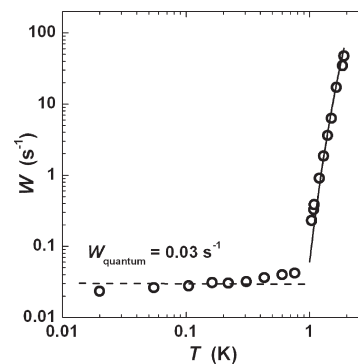


A. Morello, O.N. Bakharev, H.B. Brom, L.J. de Jongh

Polyhedron 22 (2003) 1745

Quantum tunnelling of magnetization in Mn_{12-ac} studied by ⁵⁵Mn NMR

We present an ultra-low temperature study (down to *T* = 20 mK) of the nuclear spin-lattice relaxation (SLR) in the ⁵⁵Mn nuclei of the molecular magnet Mn_{12-ac}.

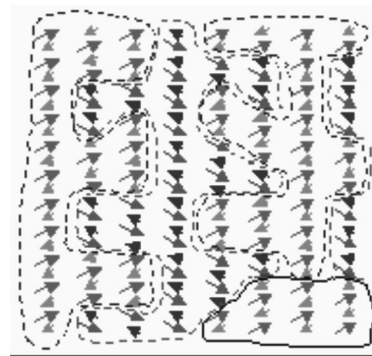


Stephen J. Etzkorn, Wendy Hibbs, Joel S. Miller, Arthur J. Epstein

Polyhedron 22 (2003) 1751

Anomalous cluster glass behavior in a quasi-one-dimensional organic-based magnet

The spin glass state of the quasi-one-dimensional (1D) organic-based magnet $[\text{MnTPP}]^+[\text{TCNE}]^- \cdot 2(1,3\text{-C}_6\text{H}_4\text{Cl}_2)$ was investigated with both a.c. and d.c. measurements. The results show the material forms quasi-1D spin clusters with a fractal dimensionality ranging from 0.8 to 1.5.

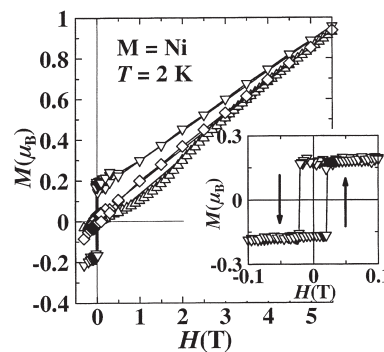


Junichi Nishijo, Akira Miyazaki, Toshiaki Enoki

Polyhedron 22 (2003) 1755

Weak-ferromagnetism in molecular magnets based on transition metal complexes of crown thioether

New molecular based magnets $\text{M}(\text{9S3})_2\text{-}[\text{Ni}(\text{bdt})_2]_2$ ($\text{M} = \text{Ni}, \text{Co}$; $\text{9S3} = 1,4,7\text{-trithia-cyclononane}$, $\text{bdt} = 1,2\text{-benzenedithiolate}$) show weak ferromagnetism with remanent magnetization $M_{\text{REM}} = 0.2 \mu_{\text{B}}$ and coercive force $H_{\text{C}} = 200 \text{ Oe}$ for $\text{M} = \text{Ni}$ and $M_{\text{REM}} = 0.01 \mu_{\text{B}}$ and $H_{\text{C}} = 10 \text{ Oe}$ for $\text{M} = \text{Co}$, respectively. The crystal structures, magnetic susceptibilities and the origin of the weak ferromagnetism were investigated.

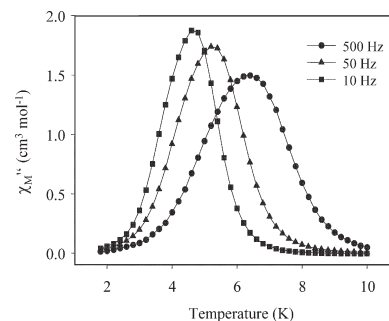


Nicole E. Chakov, Khalil A. Abboud, Lev N. Zakharov, Arnold L. Rheingold, David N. Hendrickson, George Christou

Polyhedron 22 (2003) 1759

Reaction of $[\text{Mn}_{12}\text{O}_{12}(\text{O}_2\text{CR})_{16}(\text{H}_2\text{O})_4]$ single-molecule magnets with non-carboxylate ligands

The site-specific incorporation of non-carboxylate organic ligands onto the Mn_{12} core has been accomplished. The title compound has eight benzenesulfonate in the eight axial positions. The complex is a single-molecules magnet (SMM).

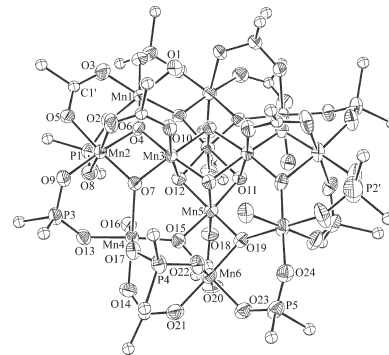


Jonathan T. Brockman, Khalil A. Abboud, David N. Hendrickson, George Christou

Polyhedron 22 (2003) 1765

A new family of Mn_{12} single-molecule magnets: replacement of carboxylate ligands with diphenylphosphinates

The new $[\text{Mn}_{12}\text{O}_{12}(\text{O}_2\text{CPh})_7(\text{O}_2\text{PPh}_2)_9(\text{H}_2\text{O})_4]$ mixed ligand complex has been prepared. Structural characterization reveals two abnormally oriented $\text{Mn}(\text{III})$ Jahn-Teller elongation axes. The complex has $S = 10$ ground state and exhibits single-molecule magnetism behavior.

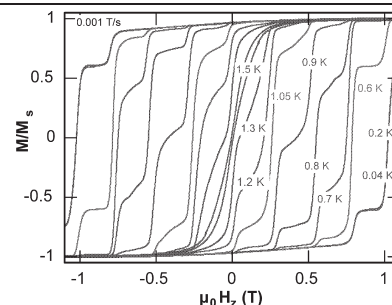


Euan K. Brechin, Monica Soler, George Christou, James Davidson, David N. Hendrickson, Simon Parsons, Wolfgang Wernsdorfer

Polyhedron 22 (2003) 1771

Magnetization tunneling in an enneanuclear manganese cage

Single-crystal magnetic measurements on the SMM $[\text{Mn}_9\text{O}_7(\text{OAc})_{11}(\text{thme})_{11}(\text{py})_3(\text{H}_2\text{O})_2]$ reveal time- and temperature-dependent hysteresis loops containing steps at regular intervals of field. DC and AC relaxation measurements confirm magnetization tunnelling in the lowest energy zero-field split component of the ground state.

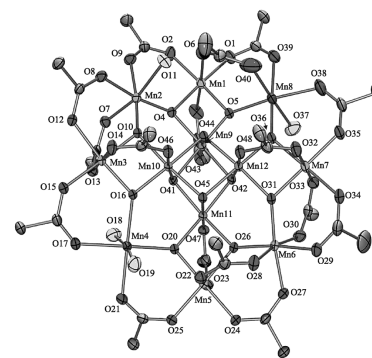


Mònica Soler, Wolfgang Wernsdorfer, Khalil A. Abboud, David N. Hendrickson, George Christou

Polyhedron 22 (2003) 1777

Single-molecule magnetism behavior of $[\text{Mn}_{12}\text{O}_{12}(\text{O}_2\text{CR})_{16}(\text{H}_2\text{O})_4]^{2-}$ salts

Convenient methods have been devised for the two-electron reduction of the Mn_{12} family of single-molecule magnets (SMMs). The resulting $[\text{Mn}_{12}]^{2-}$ compounds possess $S=10$ ground states and still retain the SMM property of the Mn_{12} and $[\text{Mn}_{12}]^{-}$ analogues. The Mn_{12} family of SMMs has now been isolated and studied in three different oxidation states.

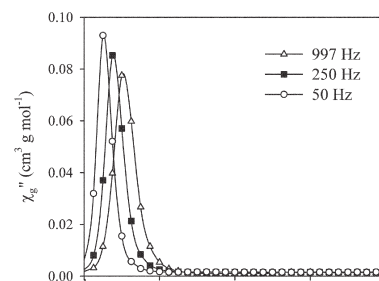


Mònica Soler, Wolfgang Wernsdorfer, Ziming Sun, Daniel Ruiz, John C. Huffman, David N. Hendrickson, George Christou

Polyhedron 22 (2003) 1783

New example of Jahn-Teller isomerism in $[\text{Mn}_{12}\text{O}_{12}(\text{O}_2\text{CR})_{16}(\text{H}_2\text{O})_4]$ complexes

The faster- and slower-relaxing forms of $[\text{Mn}_{12}\text{O}_{12}(\text{O}_2\text{CCH}_2\text{Bu}')_{16}(\text{H}_2\text{O})_4]$ have been obtained in 100% purity. These Jahn-Teller isomers crystallize isomorphously, and differ only in the orientation of one Mn(III) Jahn-Teller axis, and in the identity of one solvent molecule of crystallization. Hysteresis loops are reported for both forms, the first time for a pure single crystal of the faster-relaxing form.

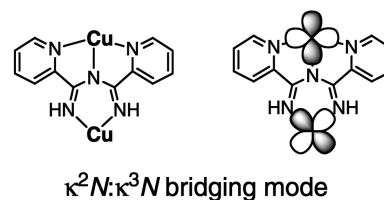


Takashi Kajiwara, Asako Kamiyama, Tasuku Ito

Polyhedron 22 (2003) 1789

Ferromagnetic interactions through control of the bridging geometry

A novel trinuclear Ni(II)-Cu(II)-Ni(II) complex and three Cu(II)-Cu(II), Ni(II)-Cu(II), and Mn(II)-Cu(II) alternating chain complexes were synthesized using the complexed ligand $[\text{Cu}(\text{btpap})_2]$ which acts as a bis-*mer*-tridentate ligand ($\text{btpap}^- = 2,4$ -bis(2-pyridyl)-1,3,5-triazapentanedienate). In the multinuclear complexes, ferromagnetic interaction operates between two adjoining metal ions connected by btpap^- in a $\kappa^2\text{N}:\kappa^3\text{N}$ bridging fashion with local C_2 symmetry.

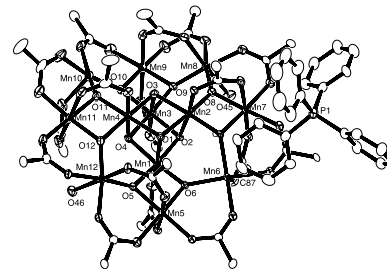


Takayoshi Kuroda-Sowa, Tadahiro Nogami, Hisashi Konaka, Masahiko Maekawa, Megumu Munakata, Hitoshi Miyasaka, Masahiro Yamashita

Polyhedron 22 (2003) 1795

Synthesis, crystal structure and magnetic properties of novel Mn_{12} single-molecule magnets with thiophenecarboxylate, $[Mn_{12}O_{12}(O_2CC_4H_3S)_{16}(H_2O)_4]$, and its tetraphenylphosphonium salt

The preparation and characterization are reported for novel Mn_{12} SMMs having thiophenecarboxylate bridges, $[Mn_{12}O_{12}(O_2CC_4H_3S)_{16}(H_2O)_4]$ (**1**), and its PPh_4 salt (**2**). The structure analysis of **2** revealed that there are two five-coordinated Mn ions, one of which is assigned to a Mn^{II} ion being in the vicinity of the tetraphenylphosphonium cation. Both complexes exhibit out-of-phase ac magnetic susceptibility signals indicating that they are SMMs.

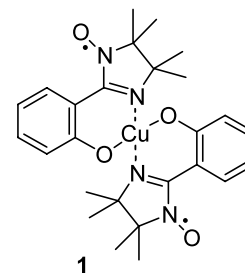


Koichiro Tanaka, Masatoshi Kozaki, Daisuke Shiomi, Kazunobu Sato, Takeji Takui, Keiji Okada

Polyhedron 22 (2003) 1803

Synthesis and magnetic properties of an iminonitroxide-substituted phenolate–Cu complex

A novel spin-chelate **1** was prepared and its magnetic properties were investigated. The complex **1** had a distorted square-planar geometry. The temperature dependence of the $\chi_p T$ values was analyzed using a three-spin model giving two magnetic parameters, $J/k_B = +250$ K and $\theta/k_B = -17$ K. These ferro- and antiferromagnetic interactions were assigned as an intramolecular Cu–iminonitroxide interaction and an intermolecular short-contact interaction, respectively.

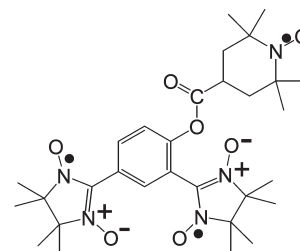


Chika Kaneda, Daisuke Shiomi, Kazunobu Sato, Takeji Takui

Polyhedron 22 (2003) 1809

A stable organic triradical with truncated π -conjugation as a model for single-component organic molecule-based ferrimagnetics

An organic triradical has been synthesized as a building block for ‘single-component ferrimagnets.’ Perturbation analyses of the solution-phase ESR spectra reveal that the triradical is characterized by two types of intramolecular exchange interactions; one is much larger than hyperfine interactions and the other is comparable to them.

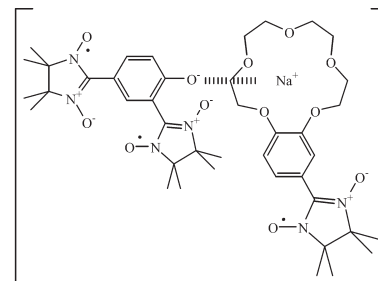


Yuki Kanzaki, Daisuke Shiomi, Kazunobu Sato, Takeji Takui

Polyhedron 22 (2003) 1817

Organic heterospin-composite systems based on supramolecular crystal engineering

A supramolecular crystal designing for organic ferrimagnets is presented. A ternary complex of a biradical anion and a Na^+ -crown-ether derivative of monoradical has been synthesized. The ground state spin multiplicity of the constituent biradical anion and the magnetic properties of the complex have been examined by ESR and magnetic susceptibility measurements.

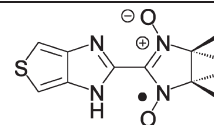


Hideaki Nagashima, Hidenari Inoue, Naoki Yoshioka

Polyhedron 22 (2003) 1823

Synthesis, solution ESR spectra, and solid-state magnetic property of thieno[3,4-*d*]imidazol-2-yl nitronyl nitroxide

A new nitronyl nitroxide derivative carrying thieno[3,4-*d*]imidazole ring was designed and synthesized. It was stable in a solid state but unstable in organic solvents. Solution ESR spectra showed that small spin densities locate on the four methyl groups and the thieno[3,4-*d*]imidazole ring. Magnetic susceptibility measurement showed that antiferromagnetic interaction is dominant which could be fitted to the Bonner–Fisher model with $J = -8.8 \text{ cm}^{-1}$.

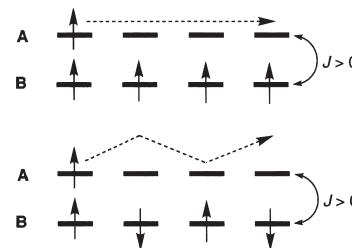


Akihiro Ito, Masashi Urabe, Kazuyoshi Tanaka

Polyhedron 22 (2003) 1829

Molecular design toward spin-polarized nano-wire: oligomer model study

In order to investigate the possibility of spin-polarized conducting polymers, quantum chemical calculations were performed for oligomer model compounds of some promising polymers carrying spin-containing units. Upon one-electron oxidation, it was confirmed that the high-spin-correlation takes place for 2-site model compounds. For 3-site and 4-site model compounds, the spin-correlation was found to be strongly dependent on the oxidation number and the molecular structure.

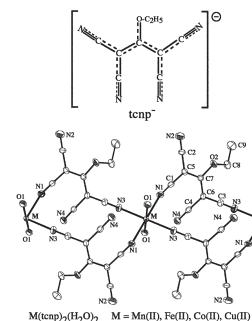


Franck Thétiot, Smail Triki, Jean Sala Pala

Polyhedron 22 (2003) 1837

Polynitriles as ligands: new coordination polymers with the 1,1,3,3-tetracyano-2-ethoxypropenide (tcnp⁻) bridging ligand

New series of mono-dimensional polynitrile-transition metal compounds, of formula $[M(\text{tcnp})_2(\text{H}_2\text{O})_2]$ ($M = \text{Mn}^{\text{II}}$, **1**; Fe^{II} , **2**; Co^{II} , **3** and Cu^{II} , **4**; $\text{tcnp}^- = [(\text{NC})_2\text{CC}(\text{OEt})\text{C}(\text{CN})_2]^-$ = 1,1,3,3-tetracyano-2-ethoxypropenide anion) have been synthesized and found to contain mono-dimensional chains of 16-membered dimetallacycles with μ_2 -bridging tcnp ligand.

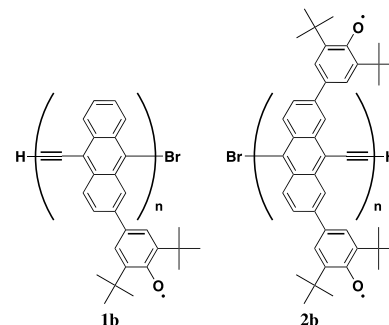


Takashi Kaneko, Takahisa Makino, Hiroshi Miyaji, Akihisa Onuma, Masahiro Teraguchi, Toshiki Aoki

Polyhedron 22 (2003) 1845

A poly(9,10-anthryleneethynylene)-based polyradical designed to be a ladder-like ferromagnetic spin coupling network

Poly(9,10-anthryleneethynylene)s-based polyradicals were synthesized from anthracene derivatives substituted with one (**1b**) or two (**2b**) phenol residues at the β -position. The statistical simulation of the ground spin states supported that the average ground state spin quantum number of **2b** ($S = 5/2$) became larger than that of **1b** ($S = 2/2$) at the same spin concentration because **2b** consists of ladder-like spin coupling network.

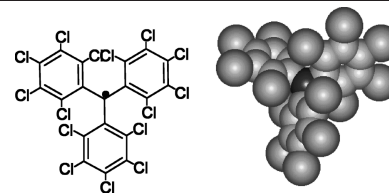


I. Ratera, D. Ruiz-Molina, C. Sporer, S. Marcen, S. Montant, J.-F. Létard, E. Freysz, C. Rovira, J. Veciana

Polyhedron 22 (2003) 1851

Nonlinear optical properties of open-shell polychlorotriphenylmethyl radicals

The second-order nonlinear optical (SONLO) response of a series of the highly chemically and thermally stable polychlorotriphenylmethyl monoradicals has been studied by Hyper-Rayleigh Scattering. These radicals exhibit relatively high nonlinear optical (NLO) responses. Such high values have been studied in terms of the open shell character and their super octupolar nature. The redox properties of the radicals have allowed to establish a redox based NLO molecular switching array.

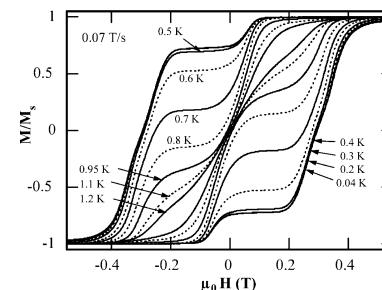


En-Che Yang, Nicholas Harden, Wolfgang Wernsdorfer, Lev Zakharov, Euan K. Brechin, Arnold L. Rheingold, George Christou, David N. Hendrickson

Polyhedron 22 (2003) 1857

Mn₄ single-molecule magnets with a planar diamond core and $S = 9$

Three Mn₄ single-molecule magnets, [Mn₄(hmp)₆(NO₃)₂(MeCN)₂](ClO₄)₂·2MeCN (**3**), [Mn₄(hmp)₆(NO₃)₄](MeCN) (**4**), and [Mn₄(hmp)₄(acac)₂(MeO)₂](ClO₄)₂·2MeOH (**5**), are prepared (hmp⁻ is the anion of 2-hydroxymethylpyridine). Crystal and molecular structures of these three complexes have been determined by means of X-ray diffraction studies. The magnetic properties of these three complexes are characterized by dc and alternating current susceptibility data. The magnetization hysteresis loops of complexes **3** and **4** show clear step features that result from quantum tunneling of magnetization.

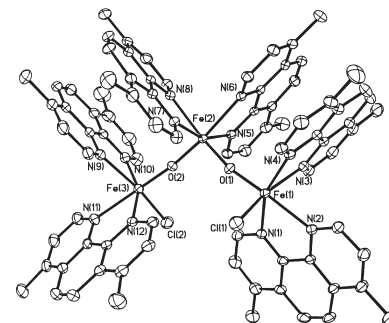


Evan M. Rumberger, Stephen Hill, Rachel S. Edwards, Wolfgang Wernsdorfer, Lev N. Zakharov, Arnold L. Rheingold, George Christou, David N. Hendrickson

Polyhedron 22 (2003) 1865

Search for new iron single-molecule magnets

A detailed study of the magnetic properties of the trinuclear half-integer spin iron complex, [Fe₃O₂Cl₂(4,7-Me-phen)₆](BF₄)₃, was undertaken. High frequency EPR and low temperature magnetometry (millikelvin) experiments were performed to determine if this complex functions as a single-molecule magnet.

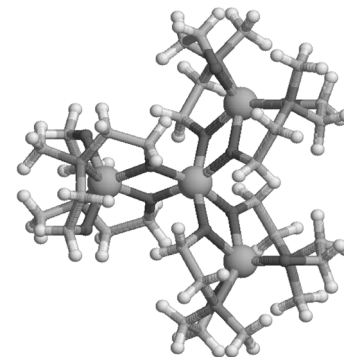


Jens Kortus, Mark R. Pederson, Tunna Baruah, N. Bernstein, C.S. Hellberg

Polyhedron 22 (2003) 1871

Density functional studies of single molecule magnets

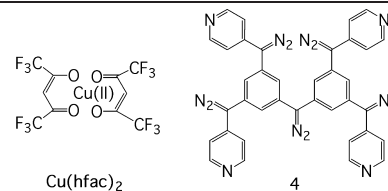
A density functional theory based method for the calculation of the second-order magnetic anisotropy parameters of single molecule magnets is reviewed. We use this method to predict the magnetic anisotropy parameters for Mn₁₂-acetate, Mn₁₀, Co₄, Fe₄, Cr₁ and V₁₅ in excellent agreement with available experimental data.



Satoru Karasawa, Noboru Koga*Polyhedron* 22 (2003) 1877

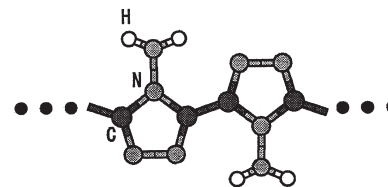
Magnetic behaviors after irradiation of assemblies consisting of bis(hexafluoroacetylacetonato)copper(II) and tetrapyridylpentadiazo compound in frozen solution

Magnetic properties after irradiation of the mixture of $\text{Cu}(\text{hfac})_2$ and **4** in MTHF/ CH_2Cl_2 solutions by 1:2, 1:1, and 2:1 ratios were investigated by SQUID. In the a.c. magnetic susceptibility measurement of the 2:1 mixture, the frequency dependence of peak-top temperature of χ' and χ'' suggested that its magnetic behavior was spin-glass like.

**Ryotaro Arita, Y. Suwa, K. Kuroki, H. Aoki***Polyhedron* 22 (2003) 1883

Possible flat-band ferromagnetism in an organic polymer

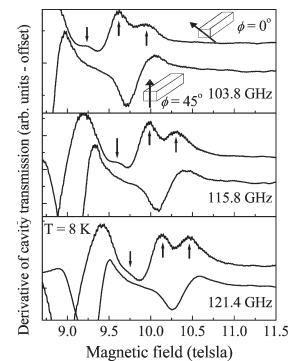
We propose that a polymer of five-membered rings, polyaminotriazole, can exhibit itinerant ferromagnetism.

**S. Hill, R.S. Edwards, J.M. North, K. Park, N.S. Dalal***Polyhedron* 22 (2003) 1889

Environmental factors influencing EPR in $\text{Mn}_{12}\text{-Ac}$ and Fe_8Br

from crystals of the $S = 10$ single molecule magnets (SMM's) $\text{Mn}_{12}\text{-Ac}$ and Fe_8Br , using a resonant cavity-based system over 1.5–75 K range. The observed lineshape and line position changes have been theoretically interpreted in terms of intermolecular spin-spin interactions (dipolar and exchange) as well as distribution in g -values and crystal-field parameters. For $\text{Mn}_{12}\text{-Ac}$, a pronounced modulation of the EPR lineshapes under transverse applied field suggests the existence of a ligand-disorder-induced anisotropy, providing a new mechanism for the quantum tunneling of magnetization in these SMM's.

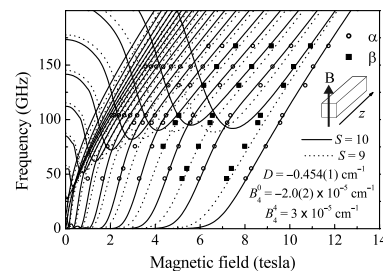
Variable-frequency (40–200 GHz), distortion-free, EPR spectra had been obtained

**S. Hill, R.S. Edwards, J.M. North, S. Maccagnano, N.S. Dalal***Polyhedron* 22 (2003) 1897

On the origin of anomalous EPR peaks observed in $\text{Mn}_{12}\text{-Ac}$

the anomalous electron paramagnetic resonance (EPR) transitions first observed in $\text{Mn}_{12}\text{-Ac}$. The most dominant of these transitions manifest themselves as an extra series of EPR absorption peaks for spectra obtained with the DC field applied within the hard magnetic plane. Our temperature- and frequency-dependent measurements demonstrate unambiguously that these anomalous EPR absorptions vanish as the temperature tends to zero, thereby indicating that they correspond to transitions from an excited state of the molecule. These findings compare favorably with available neutron scattering data.

We present a detailed investigation of the temperature and frequency dependence of

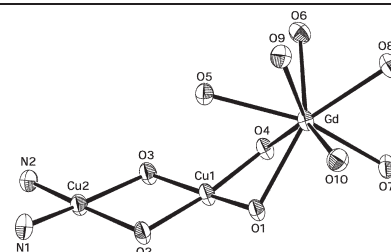


Masaaki Ohba, Nobuto Ohtsubo,
Takuya Shiga, Masatomi Sakamoto,
Hisashi Okawa

Polyhedron 22 (2003) 1905

Synthesis, structure and magnetic properties
of a linear Cu(II)Cu(II)Gd(III) complex

A dimetallic trinuclear Cu(II)₂Gd(III) complex, [Cu₂(L)][Gd(hfac)₃] (H₄L = 3,3'-(1,2-ethanediyldinitrilo)bis(1-*o*-hydroxyphenyl-1-butaneonato)) has been synthesized, and structurally and magnetically characterized. [Cu₂(L)] unit coordinates to [Gd(hfac)₃] through two phenolate oxygen atoms to afford a linear Cu(II)–Cu(II)–Gd(III) system. Its magnetic property is dominated by the antiferromagnetic interaction between two Cu²⁺ ions, and the Gd³⁺ ion behaves like a magnetically isolated ion.

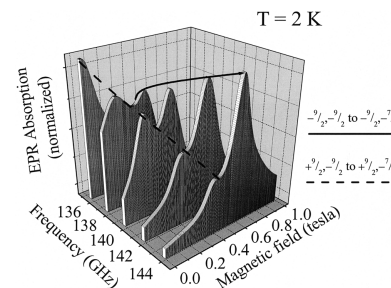


R.S. Edwards, S. Hill, S. Bhaduri, N.
Aliaga-Alcalde, E. Bolin, S. Maccagnano, G.
Christou, D.N. Hendrickson

Polyhedron 22 (2003) 1911

A comparative high frequency EPR study of
monomeric and dimeric Mn₄ single-molecule
magnets

In this study, a comparative study of single
crystal high-frequency electron paramagnetic
resonance (EPR) is presented for
monomeric and dimeric Mn₄ complexes
where, in the case of the latter, intra-dimer
exchange interactions are known to significantly
alter the low temperature quantum
behavior.

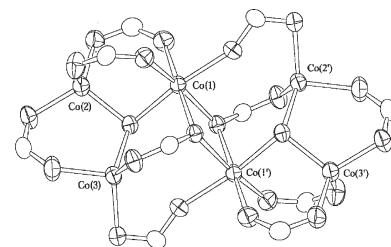


Hitoshi Kumagai, Yoshimi Oka, Satoshi
Kawata, Masaaki Ohba, Katsuya Inoue,
Mohamedally Kurmoo, Hisashi Ôkawa

Polyhedron 22 (2003) 1917

Hydrothermal synthesis, crystal structure
and characterization of a new hexanuclear
cobalt(II) complex comprised of octahedral
and tetrahedral cobalt ions

A new hexanuclear Co(II) complex,
[Co₆(OH)₂(L)₁₀] (L = phenylcinnamate) was
synthesized and characterized. [Co₆(OH)₂(L)₁₀]
consists of two edge-sharing octahedral {CoO₆}
and tetrahedral {CoO₄} units linked through
 μ -carboxylate ligands and μ -hydroxide ions.

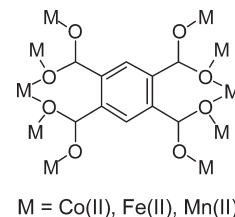


Hitoshi Kumagai, Karena W. Chapman,
Cameron J. Kepert, Mohamedally Kurmoo

Polyhedron 22 (2003) 1921

Binary metal(II)–pyromellitate coordination
polymers, M₂(pm) (M = Co, Fe, Mn): syn-
thesis, structures and magnetic properties

The hydrothermally prepared binary M₂^{II}-
pyromellitate (M = Co, Fe and Mn) exhibits
a highly compact structure consisting of an
unprecedented formation of 10 valence
bonds between each pyromellitate and the
metal ions. They are antiferromagnets ex-
cept for the cobalt salt that displays very
complex metamagnetism.

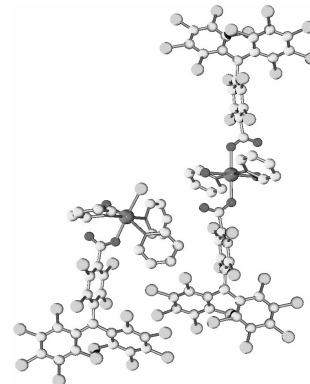


D. Maspoch, D. Ruiz-Molina, K. Wurst, C. Rovira, J. Veciana

Polyhedron 22 (2003) 1929

Synthesis, X-ray structure and magnetic properties of a unusual transition Co(II) complex with polychlorotriphenylmethyl radicals

A new cobalt(II) complex with a polychlorotriphenylmethyl radical ligand properly functionalized with a carboxylate group (PTMMC⁻), [Co(PTMMC)₂(py)₂(H₂O)₂]·[Co(PTMMC)(py)₃(H₂O)(Cl)]₂·2py·2THF (**3**), has been synthesized and characterized including single-crystal X-ray diffraction.

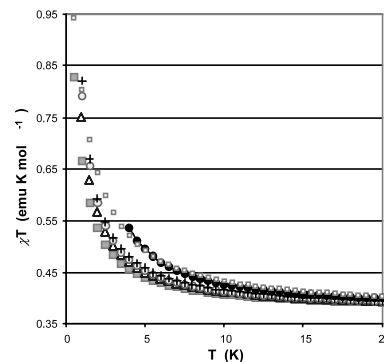


Mercè Deumal, Mike A. Robb, Juan J. Novoa

Polyhedron 22 (2003) 1935

The mechanism of the magnetic interaction in the β phase of the *p*-(nitro)phenyl nitronyl nitroxide (KAXHAS). A bottom-up study using only ab initio data

The macroscopic magnetic properties of the β phase of *p*-(nitro)phenyl nitronyl nitroxide (KAXHAS) crystal have been rationalized using a theoretical bottom-up approach, which only uses the evaluation of the microscopic interactions between pairs of radicals and the corresponding magnetic structure.

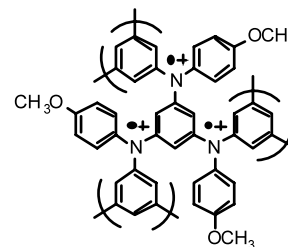


Tsuyoshi Michinobu, Jun Inui, Hiroyuki Nishide

Polyhedron 22 (2003) 1945

Preparation of non-Kekulé- and nondisjoint-type aromatic polyamines by palladium-catalyzed polycondensation and their poly(cationic radical)s

A series of triarylamine polymers were prepared by palladium-catalyzed polycondensation. Chemical oxidation of the polymer with NOPF₆ gave the corresponding polyradical, of which ESR spectrum showed a $\Delta M_s = \pm 2$ transition signal with an asymmetric fine structure.

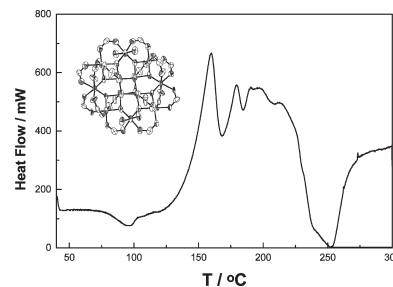


Philippe Gerbier, Daniel Ruiz-Molina, Jordi Gómez, Klaus Wurst, Jaume Veciana

Polyhedron 22 (2003) 1951

Examining the thermolysis reactions of nanoscopic Mn₁₂ single molecule magnets

The thermal behavior of three Mn₁₂ single molecule magnets [Mn₁₂O₁₂(O₂CC₆H₅)₁₆(H₂O)₄]·CH₂Cl₂·C₆H₅CO₂H **1**, [Mn₁₂O₁₂(O₂C^tBu)₁₆(H₂O)₄] **2** and [Mn₁₂O₁₂(O₂CCHCl₂)₁₆(H₂O)₄] **3** is reported. Aromatic ligands allow the complex **1** to be stable up to 300 °C whereas alkyl groups decrease drastically the domain of thermal stability for the complexes **2** and **3**. Moreover, the thermal decarboxylation of complexes **2** and **3** generates [Mn₆O₂(O₂CR)₁₀L₄] (L = H₂O, HO₂CR) complexes as characterized by single crystal X-ray diffraction when R = ^tBu.

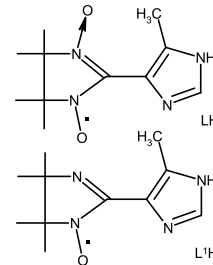


Elena Fursova, Galina Romanenko, Vladimir Iorskii, Victor Ovcharenko

Polyhedron 22 (2003) 1957

Copper(II) complexes with imidazol-4-yl derivatives of 2-imidazoline nitroxides

Copper complexes with nitronyl- and iminonitroxides containing an imidazol-4-yl substituent in the side chain have been synthesized. In the solid state, the molecules are linked by strong intermolecular N–H...O hydrogen bonds, leading to the formation of dimers, bands, or polymer layers. It has been found that antiferromagnetic exchange interactions (~ -150 to -350 cm⁻¹) are concentrated in the Cu(II)-coordinated nitroxide exchange clusters.



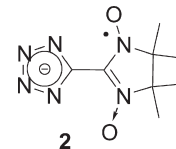
Cu(hfac)₂LH, Cu(hfac)₂L¹H,
Cu(hfac)(CF₃COO)LH,
Cu(LH)₂(NO₃)₂, Cu(L¹H)₂(NO₃)₂

Eugene V. Tretyakov, Sergey V. Fokin, Galina V. Romanenko, Victor I. Ovcharenko

Polyhedron 22 (2003) 1965

Nitronyl nitroxides containing tetrazole substituents and metal complexes with spin-labeled tetrazole

The first nitronyl nitroxides containing tetrazole substituents: sodium salt of 2-(1*H*-tetrazol-5-yl)-4,4,5,5-tetramethyl-4,5-dihydro-1*H*-imidazol-3-oxide-1-oxyl (Na(**2**)), 2-(1-methyl-1*H*-tetrazol-5-yl)-4,4,5,5-tetramethyl-4,5-dihydro-1*H*-imidazol-3-oxide-1-oxyl (**3**), and 2-(2-methyl-2*H*-tetrazol-5-yl)-4,4,5,5-tetramethyl-4,5-dihydro-1*H*-imidazol-3-oxide-1-oxyl (**4**) have been synthesized. The structures of **2–4** were confirmed by X-ray analysis.

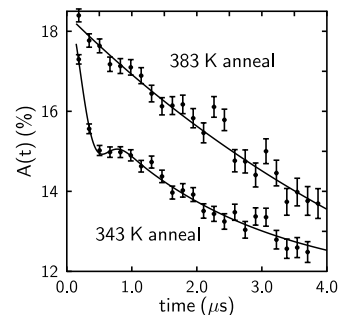


Stephen J. Blundell, Francis L. Pratt, Tom Lancaster, Ishbel M. Marshall, Christopher A. Steer, Sarah L. Heath, Jean-François Létard, Tadashi Sugano, Dragan Mihailovic, Ales Omerzu

Polyhedron 22 (2003) 1973

μ SR studies of organic and molecular magnets

Muon-spin rotation and relaxation (μ SR) experiments have been performed on a variety of novel organic and molecular magnetic systems. In these experiments, implanted muons are used to study the magnitude, distribution and dynamics of the local field at the muon site. Calculations of the spatial dependence of the dipole-field inside the unit cell are used to interpret the data and determine the muon site in certain cases. We describe and review muon experiments on nitronyl nitroxide organic ferromagnets and antiferromagnets.

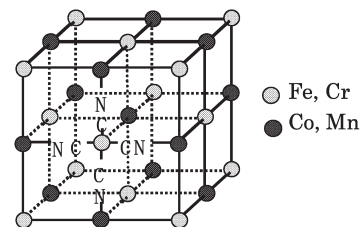


Hiroki Ishiyama, Goro Maruta, Taichi Kobayashi, Sadamu Takeda

Polyhedron 22 (2003) 1981

Hyperfine coupling of the cyanide ions and crystal water molecules of three dimensional magnetic polycyanides as studied by solid-state ¹³C- and ²H NMR

The local magnetic structures of Rb_{0.90}Mn_{1.05}[Fe(¹³CN)₆]₃·3H₂O, which exhibited a thermally induced spin phase transition near room temperature, were investigated. The hyperfine coupling of ¹³C atom of the cyanide ion and a character of the deuterated crystal water molecules were studied by solid-state ¹³C and MAS ²H NMR spectrum for various systems, i.e. Fe–CN–Mn, Fe–CN–Co and Cr–CN–Mn.



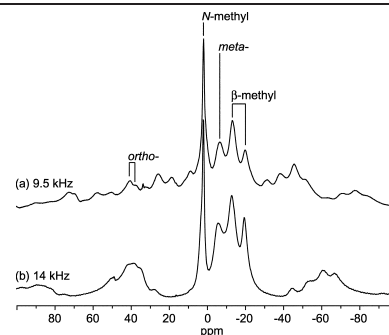
Fe(S=1/2) ↑—↓ C ≡ N—↑ Mn(S=5/2)
Hyperfine coupling of ¹³C

Goro Maruta, Sadamu Takeda, Akira Yamaguchi, Tsunehisa Okuno, Kunio Awaga

Polyhedron 22 (2003) 1989

Spin density distributions of *p*-*N*-alkylpyridinium nitronyl nitroxides studied by solid-state high-resolution NMR

Hyperfine coupling constants for protons in radical salts, *p*-MPYNN⁺I and *p*-BPYNN⁺I, were determined from the temperature dependence of ¹H MAS NMR spectra. The observed coupling constants are essentially the same as those of neutral α -aryl nitronyl nitroxide.

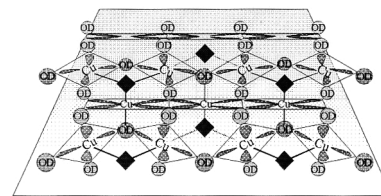


Kunio Morii, Goro Maruta, Sadamu Takeda

Polyhedron 22 (2003) 1995

Ferro- and antiferromagnetic interactions of layer-structured basic copper compounds as studied by solid-state high-resolution deuterium NMR

Magnetic local structure of a ferromagnetic layer-structured basic copper compound $\text{Cu}_2(\text{OD})_{1.96}(\text{C}_4\text{H}_6(\text{COO})_2)_{1.02} \cdot 0.07\text{D}_2\text{O}$ with dicarboxylate anion was examined by solid-state high-resolution deuterium NMR. A ferromagnetic exchange interaction $J = +71$ K within a copper chain was estimated from the temperature dependence of the isotropic shift of Magic angle spinning deuterium NMR signal of the OD^- ion.

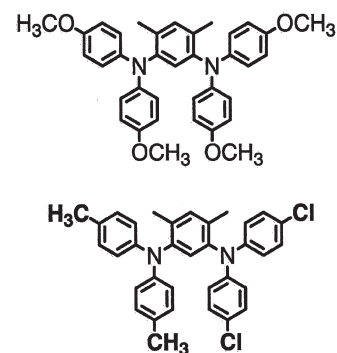


Masafumi Yano, Kentaro Aoyama, Yutaka Ishida, Masakazu Tatsumi, Kazunobu Sato, Daisuke Shiomi, Takeji Takui

Polyhedron 22 (2003) 2003

Organic high-spin and mixed-valence systems; synthesis, electrochemical and spectroscopic studies of asymmetric and symmetric tetraaryl-*m*-phenylenediamines

An asymmetric tetraaryl-1,3-phenylenediamine was designed and synthesized as a model for positively charged high-spin systems as well as for organic mixed-valence molecular systems, and their electrochemical and spectroscopic properties were examined. The stabilities of the corresponding mono- and dicationic states were also examined.

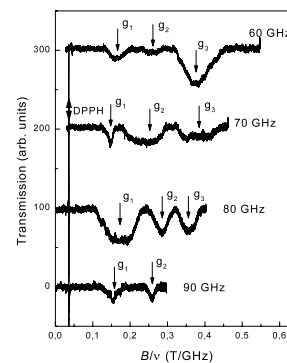


Natalia Spitsina, Sergey Demishev, Hitoshi Ohta, Susumu Okubo, Yugo Oshima, Liesbet Weckhuysen

Polyhedron 22 (2003) 2009

Magnetic properties of the fullerene organic compounds in strong magnetic fields

Magnetisation and ESR spectroscopy data for the molecular complexes $\text{C}_{60} \cdot \text{TMTSF} \cdot 2\text{CS}_2$ and $(\text{ET})_2\text{C}_{60}$ provide experimental evidence that a paramagnetic centers with the reduced *g*-factor values $g < 1$ ($g_1 = 0.43 \pm 0.03$, $g_2 = 0.27 \pm 0.02$ and $g_3 = 0.19 \pm 0.01$) control magnetic properties of these solids. Anomalous *g*-factor values may be caused by dynamic Jahn-Teller effect on the negative C_{60}^- ions, which appear as defects in crystalline structure with a weak charge transfer.

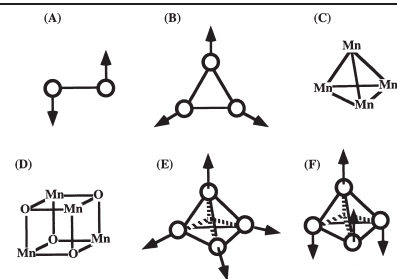


Shusuke Yamanaka, Ryo Takeda, Kizashi Yamaguchi

Polyhedron 22 (2003) 2013

Density functional study of tetrahedral manganese clusters

The spin structures of tetrahedral Mn_4 clusters are investigated by ab initio DFT computations based on generalised spin orbitals. For oxo-bridged Mn_4 , the three dimensional spin structure is found to be most stable, which is qualitatively agree with the experimentally reported effective exchange integral values of $(C_{12}H_{14}N_3OMn(II))_4 \cdot 2H_2O$.

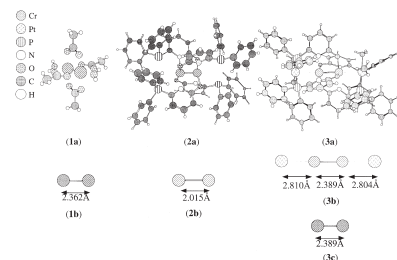


Yasutaka Kitagawa, Shuhei Nakano, Takashi Kawakami, Kazushi Mashima, Kizashi Yamaguchi

Polyhedron 22 (2003) 2019

Magnetic effective density functional studies on electronic states of $Cr_2(pyphos)_4$ and $Pt_2Cr_2(pyphos)_4(CH_3)_4$

The effective exchange integral (J_{ab}) values between chromium ions in the aligned metal complexes; $Cr_2(pyphos)_4$ and $Pt_2Cr_2(pyphos)_4(CH_3)_4$ were investigated theoretically.

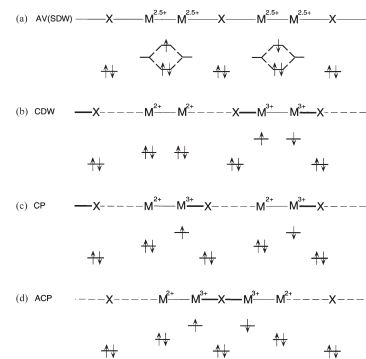


Shuhei Nakano, Yasutaka Kitagawa, Takashi Kawakami, Kizashi Yamaguchi

Polyhedron 22 (2003) 2027

Hybrid DFT study of electronic structure on quasi-one-dimensional halogen-bridged binuclear metal complexes (MMX)

The electronic structure of quasi-one-dimensional halogen-bridged binuclear metal complex $Ni_2(dta)_4I$ ($dta = CH_3CS_2^-$) was investigated by hybrid density functional theory. UB3LYP was successfully applied to reproduce averaged-valence spin density wave state. The magnetic interactions between Ni dimers were estimated by calculating effective exchange integrals (J_{ab}) using $Ni_2(dta)_4I$ dimer and tetramer models. Calculated J values were consistent with that of experimental results.

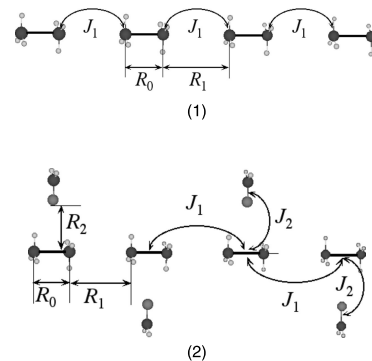


Takeshi Taniguchi, Shuhei Nakano, Takashi Kawakami, Kizashi Yamaguchi

Polyhedron 22 (2003) 2039

Theoretical study on pure organomagnetic conductors with model clusters

Ab initio MO and hybrid-DFT calculations have been carried out by using model clusters; **a** $[(NH_3)_2]_n^{+n}$ for pure organic conductors and **b** $[H_2NO-(NH_3)_2]_n^{+n}$ for pure organomagnetic conductors. The results have shown that these models are reliable for investigation of intrinsic electronic states of magnetic/conductive organic compounds in detail by quantum chemical methods.



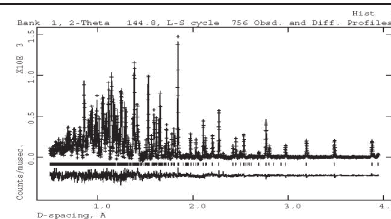
H.N. Bordallo, L. Chapon, J.L. Manson,
C.D. Ling, J.S. Qualls, D. Hall,
D.N. Argyriou

Polyhedron 22 (2003) 2045

Structural and magnetic behavior of a quasi-1D antiferromagnetic chain compound Cu(NCS)₂(pyz)

Synchrotron X-ray diffraction (XRD) and neutron powder diffraction (NPD) were used to determine the structure of Cu(NCS)₂(pyz) (pyz = pyrazine = C₄N₂H₄), which consists of a stacking of Cu-pyz-Cu

chains. While NPD measurements showed no evidence of long-range magnetic ordering, the temperature dependence of the magnetic susceptibility and magnetization suggests that the system can be adequately described on the *local* scale as a spin-1/2 antiferromagnet (AFM) chain with an intrachain exchange interaction $J/k_B = -8$ K (~ 0.7 meV). Comparison of isothermal magnetization data acquired up to 30 T at 1.6 K to a linear chain model shows excellent agreement, making this material a nearly ideal example of an isotropic Heisenberg AFM chain.

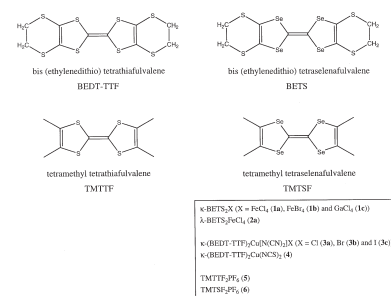


Takashi Kawakami, Takeshi Taniguchi,
Shuhei Nakano, Yasutaka Kitagawa, Kizashi Yamaguchi

Polyhedron 22 (2003) 2051

Theoretical studies on magnetic interactions in many types of organic donor salts: BEDT-TTF, BETS, TMTTF and TMTSF

Intermolecular magnetic interaction in some organic superconductive crystals were studied theoretically by using ab initio MO and DFT methods. For this purpose we employed κ -BETS₂FeCl₄ and λ -BETS₂FeCl₄ crystals for BETS salts; κ -(BEDT-TTF)₂Cu[N(CN₂)]X (X = Cl, Br and I) and κ -(BEDT-TF)₂Cu(NCS)₂ crystals for BEDT-TTF salts; TMTTF₂PF₆ and TMTSF₂PF₆ crystals for TMTTF and TMTSF salts.

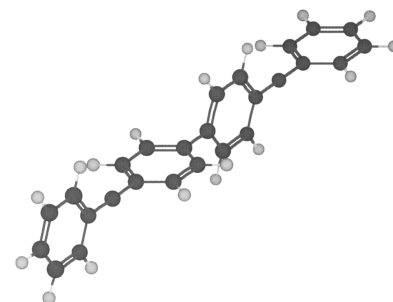


Mitsuo Shoji, Takeshi Taniguchi, Takashi Kawakami, Kizashi Yamaguchi

Polyhedron 22 (2003) 2067

Hybrid density-functional theory studies on stable polycarbenes

Electronic and magnetic stable carbene-bis(9-(10-phenyl)anthryl)carbene and its model carbenes stabilized by aromatic rings are investigated by ab initio MO and crystal orbital calculations. Magnetic interactions of model carbenes are varied as the conformational changes of the aromatic rings and are studied theoretically.

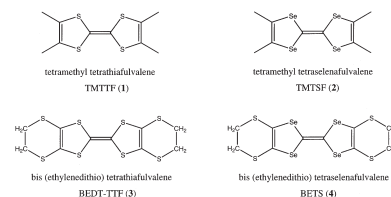


Kizashi Yamaguchi, Takashi Kawakami,
Takeshi Taniguchi, Shuhei Nakano,
Yasutaka Kitagawa, Hidemi Nagao,
Tadafumi Ohsaku, Ryo Takeda

Polyhedron 22 (2003) 2077

Theoretical studies of molecule-based magnetic conductors

In order to elucidate electronic and magnetic properties in the organo magnetic superconductors composed of donors (1–3), effective exchange integrals are calculated by ab initio hybrid DFT method. These values are numerically reproduced by using various model Hamiltonians.

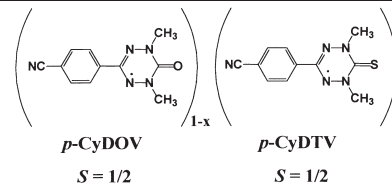


K. Mukai, M. Yanagimoto, S. Tanaka, M. Mito, T. Kawae, K. Takeda

Polyhedron 22 (2003) 2091

Heat capacity study of the doping effect of paramagnetic impurity in organic spin-Peierls system: *p*-CyDOV radical crystal

Heat capacity studies were performed for the doped verdazyl radical crystals, (*p*-CyDOV)_{1-x}(*p*-CyDTV)_x ($x = 0, 0.01, \text{ and } 0.07$), to clarify the effect of magnetic impurity (*p*-CyDTV) on the spin-Peierls transition ($T_{SP} = 15.0 \text{ K}$) of *p*-CyDOV radical crystal. The antiferromagnetic transitions were observed at $T_N = 0.135, 0.290 \text{ and } 0.164 \text{ K}$ for the crystals with $x = 0, 0.01, \text{ and } 0.07$, respectively.

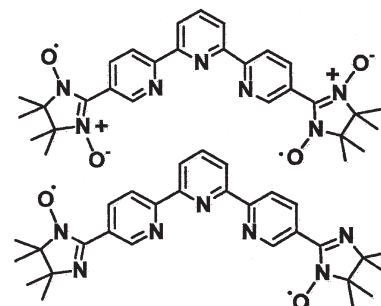


Giorgio Zoppellaro, Anela Ivanova, Volker Enkelmann, Ahmed Geies, Martin Baumgarten

Polyhedron 22 (2003) 2099

Synthesis, magnetic properties and theoretical calculations of novel nitronyl nitroxide and imino nitroxide diradicals grafted on terpyridine moiety

The first example of intramolecular ferromagnetic interactions through terpyridine based biradicals is reported.

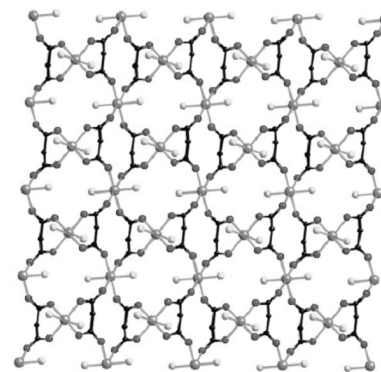


Catalina Ruiz-Pérez, Yolanda Rodríguez-Martín, María Hernández-Molina, Fernando S. Delgado, Jorge Pasán, Joaquín Sanchiz, Francesc Lloret, Miguel Julve

Polyhedron 22 (2003) 2111

Malonic acid: a multi-modal bridging ligand for new architectures and properties on molecule-based magnets

We show how the design of one-, two- and three-dimensional materials can strongly benefit from the use of crystal engineering techniques, which can give rise to structures of different shapes, and how these differences can give rise to different properties. We will focus on the networks constructed by assembling malonate ligands and metal centres.

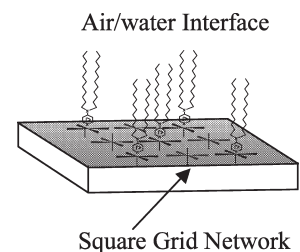


Jeffrey T. Culp, Ju-Hyun Park, Isa O. Benitez, Mark W. Meisel, Daniel R. Talham

Polyhedron 22 (2003) 2125

Two applications of metal cyanide square grid monolayers: studies of evolving magnetic properties in layered films and templating Prussian blue family thin films

A mixed-metal cyanide square grid network fabricated as a Langmuir monolayer at the air/water interface is applied in two separate studies. In the first, the magnetic properties of a monolayer, bilayer, and multiple layers are compared. In the second, the monolayer is used to provide epitaxy with bulk Prussian blue analogs.

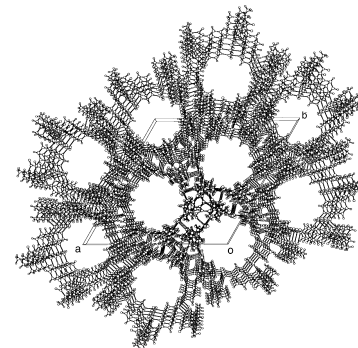


Takayuki Ishida, Junichi Omata, Takashi Nogami

Polyhedron 22 (2003) 2133

Host–guest chemistry of radical-copper wheels. A supramolecular control of magnetic exchange coupling

The ferromagnetic interaction of $[\text{CuCl}_2 \cdot (4\text{PMNN})_6]$, which is ascribed to intermolecular contacts between the nitronyl nitroxide groups, was remarkably enhanced by the guest (LiCl, NaCl, KCl and H_2O) inclusion within the tube-like cavity.

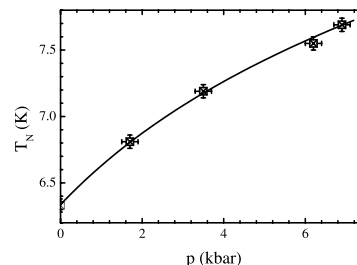


A.U.B. Wolter, Hans-Henning Klaus, F. Jochen Litterst, T. Burghardt, Andreas Eichler, Ralf Feyerherm, S. Süllow

Polyhedron 22 (2003) 2139

A pressure study of the antiferromagnetic phase of FePM_2Cl_2 (PM = pyrimidine)

We present high pressure magnetization and neutron scattering experiments on FePM_2Cl_2 (PM = pyrimidine). This material undergoes a transition into a canted antiferromagnet below $T_N = 6.3$ K. We establish the bulk modulus, the anisotropy of the compression and the pressure dependence of the antiferromagnetic transition temperature.

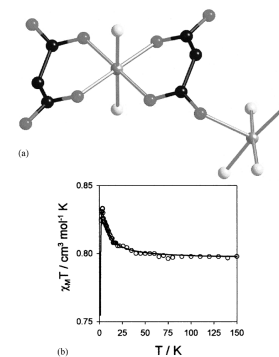


Jorge Pasán, Fernando S. Delgado, Yolanda Rodríguez-Martín, María Hernández-Molina, Catalina Ruiz-Pérez, Joaquín Sanchíz, Francesc Lloret, Miguel Julve

Polyhedron 22 (2003) 2143

Malonate-based copper(II) coordination compounds: ferromagnetic coupling controlled by dicarboxylates

Studies on structural and magnetic properties of polynuclear transition metal complexes were performed. The malonate group seems a suitable candidate. The occurrence of two carboxylate groups in the 1,3 positions allows this ligand to adopt simultaneously chelating bidentate and different carboxylato bridging modes. We have structurally and magnetically characterized several carboxylato bridged copper(II) complexes.

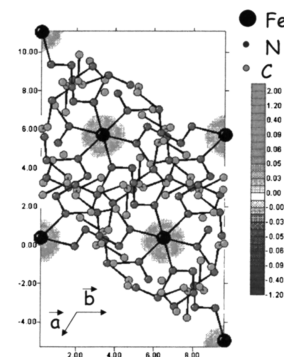


Jelena Jeftić, Béatrice Gillon, Antoine Goujon, Quiterie Nau, Arsen Gukasov, Epiphane Codjovi, François Varret

Polyhedron 22 (2003) 2155

First study of the photo-induced metastable (paramagnetic) high-spin state in a $[\text{Fe}(\text{ptz})_6](\text{BF}_4)_2$ single crystal by polarised neutron diffraction

The first spin-density map of the photo-induced metastable high-spin state in iron(II) propyltetrazole tetrafluoroborate single crystal in its $R\bar{3}$ space group has been performed by polarised neutron diffraction adapted for photophysical studies.

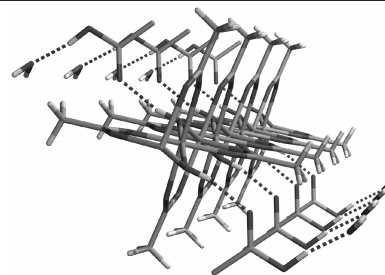


David J. Price, Stuart R. Batten, Boujemaa Moubaraki, Keith S. Murray

Polyhedron 22 (2003) 2161

Synthesis, structure and magnetism of $\{[\text{Mn}(\mu\text{-OH})(\mu\text{-OAc})_2]\cdot\text{HOAc}\cdot\text{H}_2\text{O}\}_n$ and the facilitation of long-range magnetic order through hydrogen bonding

A new manganese(III) complex $\{[\text{Mn}(\mu\text{-OH})(\mu\text{-OAc})_2]\cdot\text{HOAc}\cdot\text{H}_2\text{O}\}_n$ ($1\cdot\text{HOAc}\cdot\text{H}_2\text{O}$), whose structure consists of infinite 1D linear chains that are hydrogen-bonded to form 2D sheets, is described. The complex displays weak intra-chain antiferromagnetic coupling at higher temperatures and a magnetic phase transition, at $T_N = 6.1$ K, to an ordered antiferromagnetic phase, probably mediated by the hydrogen-bonding pathways.

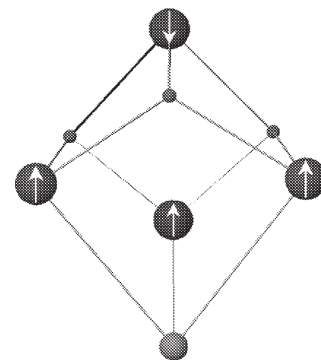


M. Evangelisti, F. Luis, F.L. Mettes, N. Aliaga, G. Aromí, G. Christou, L.J. de Jongh

Polyhedron 22 (2003) 2169

Through quantum tunneling to dipolar order: the effect of varying magnetic anisotropy in three structurally related Mn_4 molecular clusters

By means of very-low-temperature time-dependent specific heat experiments, we study the electron spin-lattice relaxation mechanisms of three Mn_4 clusters, which have same magnetic core but different anisotropy. We show that the spin-lattice relaxation rate increases when the tunneling probabilities increase, thus indicating that quantum tunneling brings the spins towards equilibrium.

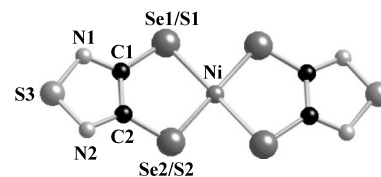


Paola Deplano, Luciano Marchiò, Maria Laura Mercuri, Luca Pilia, Angela Serpe, Emanuele F. Trogu

Polyhedron 22 (2003) 2175

New nickel dithiolene–diselenolene complexes obtained from 3,4-dichloro-1,2,5-thiadiazole. X-ray structure of $(\text{Bu}_4\text{N})_2[\text{Ni}(\text{C}_2\text{N}_2\text{S}_{2.2}\text{Se}_{0.8})_2]$

The new $(\text{Bu}_4\text{N})_2[\text{Ni}(\text{C}_2\text{N}_2\text{S}_{2.2}\text{Se}_{0.8})_2]$ redox active nickel complex (see the anion in the pictogram) and its mono-oxidation product with a mixed $\text{S}_{0.6}/\text{Se}_{0.4}$ occupancy of thiolic sulfurs in the ligand have been prepared. These species seem interesting to work as diamagnetic and paramagnetic counterions of suitable donors to prepare CT salts.

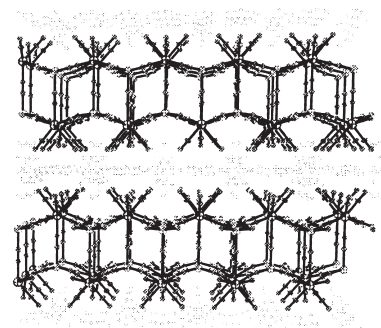


Tomasz Korzeniak, Robert Podgajny, Nathaniel W. Alcock, Krzysztof Lewiński, Maria Balanda, Tadeusz Wasiutyński, Barbara Sieklucka

Polyhedron 22 (2003) 2183

A new family of magnetic 2D coordination polymers based on $[\text{M}^{\text{V}}(\text{CN})_8]^{3-}$ ($\text{M} = \text{Mo}, \text{W}$) and pre-programmed Cu^{2+} centres

Four heterometallic 2D coordination networks have been assembled by capping $\text{Cu}(\text{II})$ centres by octacyanometalate(V) moieties. Magnetic measurements reveal long range ferromagnetic ordering with sharp phase transition at T_C in range 28–37 K and coercivity in range 30–225 Oe at liquid helium temperature ($T = 4.3$ K).



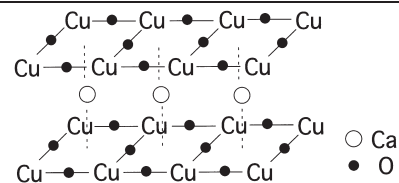
Taku Onishi, Daisuke Yamaki, Kizashi Yamaguchi

Polyhedron 22 (2003) 2191

Theoretical studies on the electronic states of electron-doped copper oxides

We have performed hybrid density functional theory calculations on infinite layer copper oxides denoted as $ACuO_2$, where A stands for the alkaline earth metal such as strontium or calcium, which are available in the strongly correlated systems such as transition metal complexes, in order to examine

the electronic states after one e-doping for the linear chain clusters such as $CuOCu$ and Cu_3O_2 . The electronic states have been clarified from view points of energy, spin and charge density populations, natural orbital analysis and the difference of density. We discuss the differences of the changes of electronic states between h-doping and e-doping.

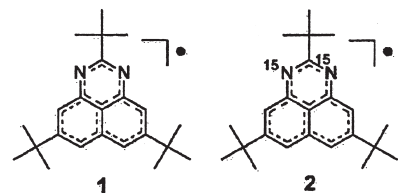


Yasushi Morita, Kozo Fukui, Shuichi Suzuki, Takashi Aoki, Shigeaki Nakazawa, Koichi Tamaki, Akira Fuyuhito, Kagetoshi Yamamoto, Kazunobu Sato, Daisuke Shiomi, Akira Naito, Takeji Takui, Kazuhiro Nakasuji

Polyhedron 22 (2003) 2199

Electronic-spin and columnar crystal structures of stable 2,5,8-tri-*tert*-butyl-1,3-diazaphenalenyl radical

Our recent studies on *tert*-butylated 1,3-diazaphenalenyl **1** as the first example of stable azaphenalenyl have encouraged us to design and synthesis of ^{15}N -incorporated 1,3-diazaphenalenyl **2** in order to elucidate the electronic structure in solid state. Nitration reaction by $K^{15}NO_3$ of 2,7-di-*tert*-butylnaphthalene has accomplished effective introduction of ^{15}N atoms and synthesis of **2**. The structure of 1,3-($^{15}N_2$)diazaphenalenyl **2** was unequivocally determined by ESR and X-ray measurements.



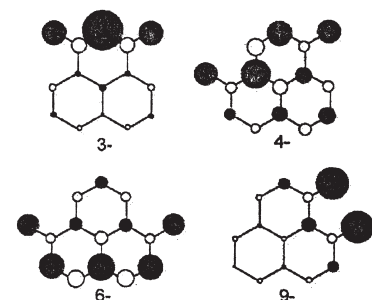
Yasushi Morita, Junya Kawai, Shinsuke Nishida, Kozo Fukui, Shigeaki Nakazawa, Kazunobu Sato, Daisuke Shiomi, Takeji Takui, Kazuhiro Nakasuji

Polyhedron 22 (2003) 2205

A novel organic neutral radical system: topological effects in oxophenalenoxyls

An oxophenalenoxyl is a phenalenyl-based neutral monoradical and has many topological isomers depending on the positions of introduced two oxygen atoms. Our experimental studies have demonstrated that the

spin-delocalized nature of the oxophenalenoxyl systems extremely depends on the topological symmetry of the introduced two oxygen atoms. The π -spin density distributions have been calculated by density functional theory, supporting the topology-dependent spin diversity nature inherent in a series of oxophenalenoxyl systems. These studies have indicated the importance of molecular topology in monoradical systems for the first time.



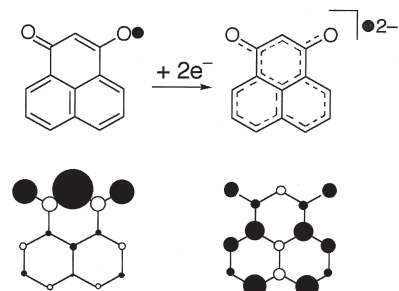
The π -spin density distributions of oxophenalenoxyl systems

Yasushi Morita, Shinsuke Nishida, Junya Kawai, Kozo Fukui, Shigeaki Nakazawa, Kazunobu Sato, Daisuke Shiomi, Takeji Takui, Kazuhiro Nakasuji

Polyhedron 22 (2003) 2209

Redox-based spin diversity: a reversible topological spin switching in oxophenalenoxyl systems

Redox-based spin diversity is the reversible topological switching nature of the spin density distribution in the spin-delocalized molecular system by controlling redox processes. 3-Oxophenalenoxyl is a neutral radical based on phenalenyl with two oxygen atoms at 1, 3 positions of phenalenyl skeleton. Our successful generation of neutral and radical dianion species and evaluation of the electronic structures clarified the redox-based spin diversity nature of 3-oxophenalenoxyl system.



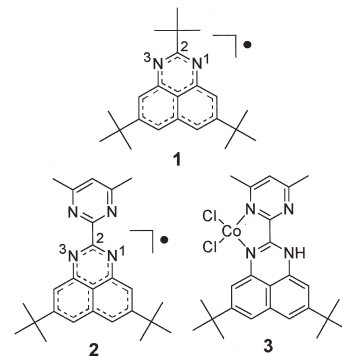
Redox-based spin diversity of 3-oxophenalenoxyl system

Yasushi Morita, Shuichi Suzuki, Kozo Fukui, Shigeaki Nakazawa, Kazunobu Sato, Daisuke Shiomi, Takeji Takui, Kazuhiro Nakasuji

Polyhedron 22 (2003) 2215

A synthetic study of metal complexes of coordinated neutral radicals based on an azaphenalenyl system

1,3-Diazaphenalenyl derivative with pyrimidine moiety **2** has been designed as a new neutral ligand on the basis of 1,3-diazaphenalenyl system **1**. As a study for the metal complexes of coordinated neutral radical, we have synthesized the metal complex coordinated diazaphenylene **3**, giving the first study on the structurally characterized metal complex based on the azaphenylene system.

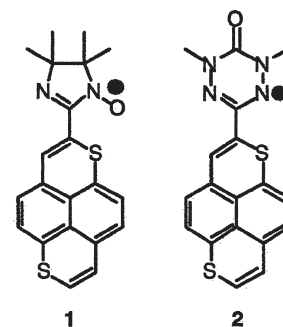


Y. Morita, E. Miyazaki, J. Kawai, K. Sato, D. Shiomi, T. Takui, K. Nakasuji

Polyhedron 22 (2003) 2219

Syntheses and spin structures of 1,6-dithiapyrene derivatives having imino nitroxide or oxoverdazyl moiety

1,6-Dithiapyrene (DTPY) derivatives with imino nitroxide or 1,5-dimethyl-6-oxoverdazyl moiety **1** and **2** have been designed and synthesized as neutral radicals. The hfccs and relative signs of the protons and nitrogen atoms for **1** and **2** were determined by ESR/ENDOR/TRIPLE measurements and DFT calculations. The unpaired electrons slightly distributed to the DTPY moieties in **1** and **2**.

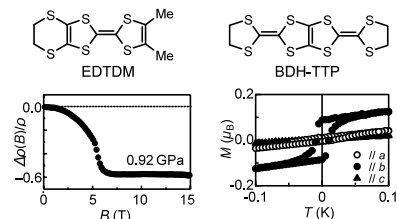


Akira Miyazaki, K. Okabe, K. Enomoto, J. Nishijo, T. Enoki, Fatima Setifi, Stéphane Golhen, Lahcène Ouahab, T. Toita, J. Yamada

Polyhedron 22 (2003) 2227

π -d Interaction-based molecular magnets

(DMET)₂FeBr₄ and (EDTDM)₂FeBr₄ show a clear correspondence of anomalies on the magnetization curves and the magnetoresistance, and a large negative magnetoresistance is also observed for the latter compound under pressure. (BDH-TTP)-[M(isoq)₂(NCS)₄] (M = Cr, Fe) show bulk magnetic order at 7.6 K, characterized as a spin-canted weak ferromagnetism.

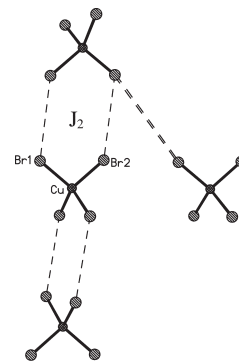


Mercè Deumal, Christopher P. Landee, Juan J. Novoa, Michael A. Robb, Mark M. Turnbull

Polyhedron 22 (2003) 2235

Through space magnetic exchange in tetrabromocuprates: theoretical considerations

Through space magnetic exchange parameters between tetrabromocuprate ions are calculated and compared with experimental values showing strong agreement.

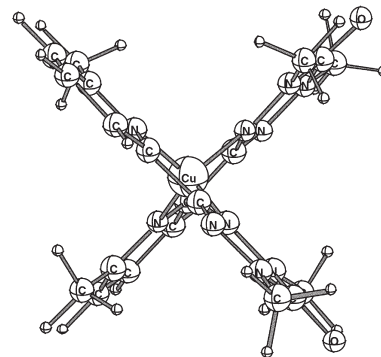


Jonathan E. Stevens,
David J.R. Brook,
Vincent W. Abeyta

Polyhedron 22 (2003) 2241

Free radical complexes of copper(I): geometry and ground state

Ab-initio DFT calculations successfully predict the ground state multiplicity, and singlet triplet separation of a copper(I)–imino-nitroxide complex and suggest that the apparently weak radical–radical interaction in a related copper(I)–verdazyl complex is a result of intermolecular interactions within the crystal structure.

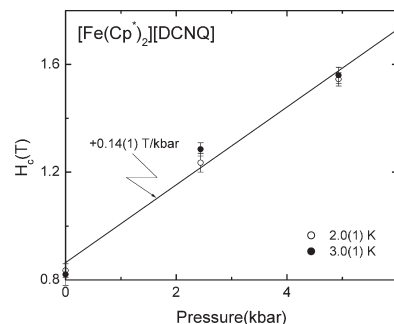


James J. Hamlin, Brett R. Beckett,
Takahiro Tomita, James S. Schilling,
William S. Tyree, Gordon T. Yee

Polyhedron 22 (2003) 2249

The effect of pressure on the magnetic properties of the molecule-based canted metamagnet decamethylferrocenium 2,3-dicyano-1,4-naphthoquinone, $\text{FeCp}^*_2[\text{DCNQ}]$

The magnetic properties of the title compound, a molecule-based metamagnet, are examined under pressures up to 5 kbar. Both T_c and H_c increase with increasing pressure suggesting stronger antiferromagnetic interactions with decreasing intermolecular distances.

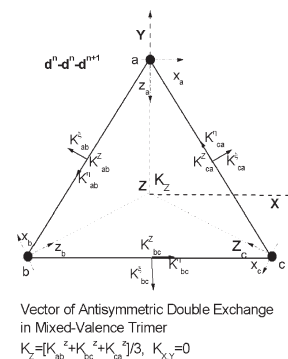


Moisey I. Belinsky

Polyhedron 22 (2003) 2253

Antisymmetric double exchange and zero-field splittings in mixed-valence clusters

The effect of an antisymmetric double exchange (AS DE) interaction in the mixed-valence (MV) dimeric d^n-d^{n+1} and trimeric $d^n-d^n-d^{n+1}$ clusters of orbitally non-degenerate ions is considered.



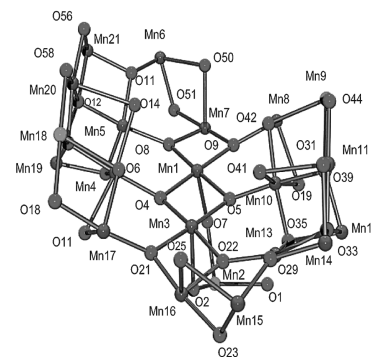
E.C. Sañudo, E.K. Brechin, C. Boskovic,
W. Wernsdorfer, J. Yoo, A. Yamaguchi,
T.R. Concolino, K.A. Abboud,
A.L. Rheingold, H. Ishimoto,
D.N. Hendrickson, G. Christou

Polyhedron 22 (2003) 2267

$[\text{Mn}_{18}]^{2+}$ and $[\text{Mn}_{21}]^{4+}$ single-molecule magnets

The synthesis and structural characterization of the two new Mn complexes $[\text{Mn}_{18}\text{O}_{14}(\text{O}_2\text{CMe})_{18}(\text{hep})_4(\text{hepH})_2(\text{H}_2\text{O})_2](\text{ClO}_4)_2$ (**1**) and $[\text{Mn}_{21}\text{O}_{16}(\text{O}_2\text{CMe})_{16}(\text{hmp})_6$

$(\text{hmpH})_2(\text{pic})_2(\text{py})(\text{H}_2\text{O})(\text{ClO}_4)_4$ (**3**) are presented, together with a detailed study of their magnetic properties. Complex **1** possesses a ground-state spin of $S = 13$, and the ground-state spin for **3** is estimated to be $S = 17/2$ or $19/2$. Both complexes **1** and **3** are new examples of single-molecule magnets (SMMs), displaying frequency-dependent out-of-phase AC signals, as well as magnetization vs. DC field hysteresis at temperatures below 1 K. Complex **1** straddles the classical/quantum interface by also displaying quantum tunneling of the magnetization (QTM).

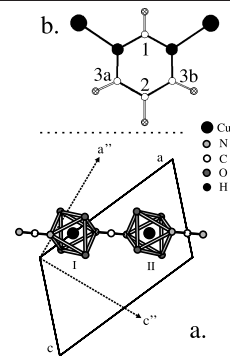


A.U.B. Wolter, P. Wzietek, F.J. Litterst, S. Söllow, D. Jérôme, R. Feyerherm, H.-H. Klauss

Polyhedron 22 (2003) 2273

^{13}C NMR on the $S = 1/2$ antiferromagnetically coupled spin chain compound $[\text{PM} \cdot \text{Cu}(\text{NO}_3)_2 \cdot (\text{H}_2\text{O})_2]_n$ (PM = pyrimidine)

We present carbon ^{13}C NMR experiments on the $S = 1/2$ antiferromagnetically coupled spin chain compound $[\text{PM} \cdot \text{Cu}(\text{NO}_3)_2 \cdot (\text{H}_2\text{O})_2]_n$ (PM = pyrimidine) at temperatures 5–120 K. In NMR spectra, we observe three pairs of double lines, assigned to three inequivalent C sites on the pyrimidine molecule $\text{C}_4\text{N}_2\text{H}_4$, splitted by the coupling to the adjacent proton spin. We observe the temperature dependence of the NMR shift, which exhibits a qualitatively different behavior for the three inequivalent C sites.

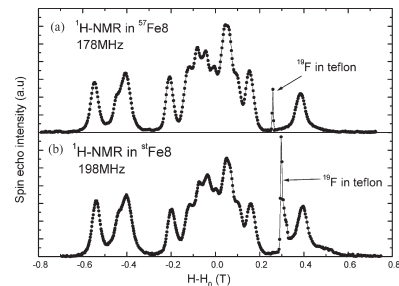


Y. Furukawa, S. Kawakami, K. Aizawa, K. Kumagai, F. Borsa

Polyhedron 22 (2003) 2277

Isotope substitution effects on spin dynamics of the molecular nanomagnet Fe8 cluster studied by NMR

We have carried out ^1H NMR at $T = 1.5$ K in both ^{57}Fe -enriched Fe8 cluster and non-enriched Fe8 cluster to investigate isotope substitution effects on magnetic properties. The field dependence of $1/T_1$ can be fitted well by using a simple model in terms of the thermal fluctuations of the total spin $S = 10$ of the cluster originating from the spin–phonon interactions. The absence of a difference of the magnetic field dependence of $1/T_1$ between the two systems indicates that the spin–phonon coupling constant is not affected by the change of mass of the isotopes in the Fe8 cluster.

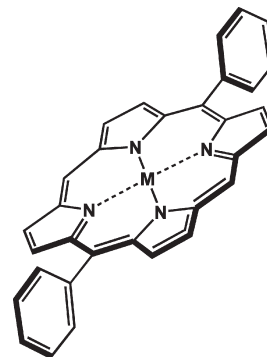


Masaru Yao, Masafumi Kamishiro, Hidenari Inoue, Naoki Yoshioka

Polyhedron 22 (2003) 2281

Synthesis and physicochemical properties of some 5,15-diarylporphyrin derivatives

meso-Diphenylmetalloporphyrins ($M = \text{Cu}, \text{VO}$) were prepared and their magnetic properties were characterized. These derivatives obeyed the Curie law and were almost identical with those of corresponding *meso*-tetraphenyl derivatives. Prepared amphiphilic diarylporphyrin showed a large red shift pattern in the visible absorption spectrum at air–water interface, compared with in the solution.



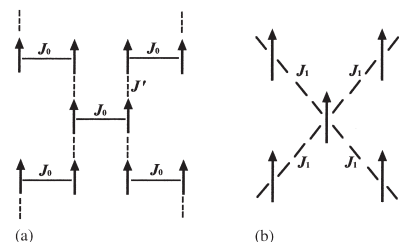
K. Takeda, M. Mito, K. Kinoshita, Miguel A. Novak, Jean Louis Tholence, André Rassat

Polyhedron 22 (2003) 2287

Pressure effects of a genuine organic crystalline ferromagnet dupeyredioxyl

We have revealed that the isothermal magnetization M of the genuine organic crystalline dupeyredioxyl (N,N' -dioxy-1,3,5,7-tetramethyl-2,6-diazaadamantane; $T_c(0) = 1.48$ K) observed below 10 K converges on the $S = 1$ Brillouin function $B_1((H + \lambda M)/k_B T)$

This fact suggests that $S = 1$ is constructed within a molecule via a strong ferromagnetic coupling between two $S = 1/2$ spins on each of the two NO moieties. Pressure effects of this compound have been studied under the hydrostatic pressure (P) up to 15 kbar. Microscopically, different from the above two ferromagnets, the pressure-induced destruction of the orthogonality of molecular orbitals associated with the two NO moieties plays an effective role in reducing the intramolecular ferromagnetic interaction J_0 .



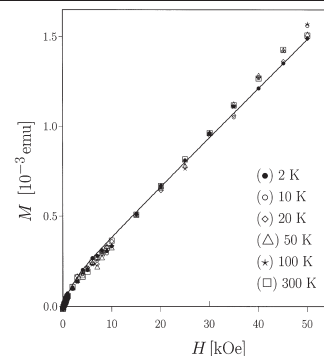
Zvonko Jagličić, Andrej Jeromen, Zvonko Trontelj, Dragan Mihailović, Denis Arčon, Maja Remškar, Aleš Mrzel, Robert Dominko, Miran Gaberšček, José M. Martínez-Agudo, Carlos J. Gómez-García, Eugenio Coronado

Polyhedron 22 (2003) 2293

Magnetic properties of MoS₂ nanotubes doped with lithium

DC magnetization measurements of lithium-doped molybdenum sulfide nano-

tubes (Li_xMoS₂, 2.2 < x < 2.5) reveal a very large, nearly linear temperature-dependent susceptibility. The susceptibility in the temperature interval from 300 to 2 K is more than 100 times larger than the susceptibility of Li metal. The $M(H)$ curves measured at several temperatures between 2 and 300 K show a very small temperature dependence. Besides the linear part of $M(H)$, the non-linear part with saturation at approximately 10 kOe can be observed. This suggests a formation of ferromagnetic clusters even at room temperature. No magnetic phase transition between 2 and 300 K has been detected.

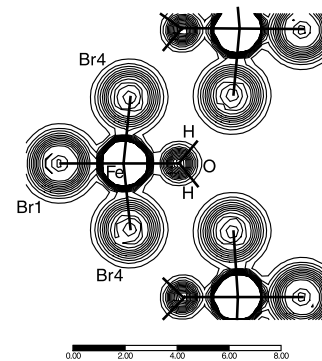


Javier Campo, Javier Luzón, Fernando Palacio, Angel Millán, Garry J. McIntyre

Polyhedron 22 (2003) 2297

Superexchange interaction enhanced through spin delocalisation in Rb₂FeBr₅·H₂O as studied by polarised neutron diffraction

Polarised neutron diffraction experiments on crystals of Rb₂FeCl₅·H₂O are reported. Experimental magnetic structure factors were analysed using a multipolar model for the magnetisation density on the iron and ligand atoms. Our results indicate that there exists an important spin transfer of 20% from the iron to the ligands. Also, a small asphericity is observed on Fe(III) ion due to the presence of the ligands. The hydrogen bridge, in the superexchange pathway Fe–Br···H–O–Fe, seems to favour the spin-density transfer from the iron through bromine, thus enhancing the magnetic interaction.

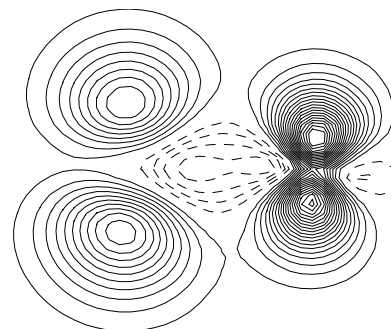


Javier Luzón, Javier Campo, Fernando Palacio, Garry J. McIntyre, Andrés E. Goeta, Christopher M. Pask, Jeremy M. Rawson

Polyhedron 22 (2003) 2301

Spin-density distribution of the high T_c p -O₂N·C₆F₄·CNSSN free radical studied by polarised neutron diffraction

Knowledge of the spin-density distribution in the dithiadiazolyl radical ring (DTDA) constitutes a major step towards the understanding of the magnetic and electronic properties of the rich magnetism of DTDA derivatives.

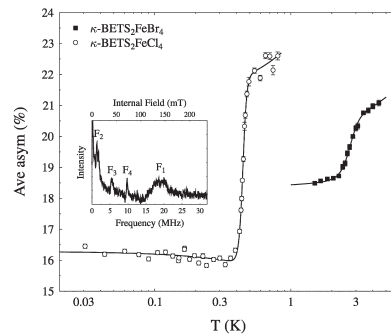


F.L. Pratt, S.J. Blundell, I.M. Marshall, T. Lancaster, S.L. Lee, A. Drew, U. Divakar, H. Matsui, N. Toyota

Polyhedron 22 (2003) 2307

μ SR studies of magnetic superconductors based on the BETS molecule

Muon spin rotation and relaxation measurements have been made on the molecular magnetic superconductors κ -BETS₂FeCl₄ and κ -BETS₂FeBr₄ and the non-magnetic molecular metals κ -BETS₂GaCl₄ and λ -BETS₂GaCl₄. When the BETS superconductors are compared with the ET-based superconductors that we have already studied using μ SR, a striking correlation was observed between T_c and λ^{-3} .

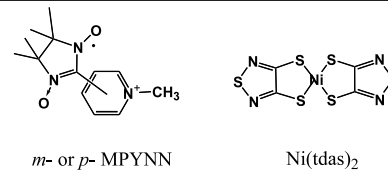


Tsune-hisa Okuno, Kazunori Kuwamoto, Wataru Fujita, Kunio Awaga, Warô Nakanishi

Polyhedron 22 (2003) 2311

Crystal structures and magnetic properties of (*m*- or *p*-MPYNN)₂Ni^{II}(tdas)₂

Novel Ni^{II}(tdas)₂ complexes, (*m*- or *p*-MPYNN)₂Ni(tdas)₂ (MPYNN = *N*-methylpyridinium α -nitronyl nitroxide and tdas = 1,2,5-thiadiazole-3,4-dithiolate), were prepared. The magnetic susceptibilities of both complexes decrease with decreasing temperature, indicating antiferromagnetic interaction within the radicals. The behavior of (*m*- and *p*-MPYNN)₂Ni(tdas)₂ was understood with the singlet–triplet model and the Curie–Weiss law.

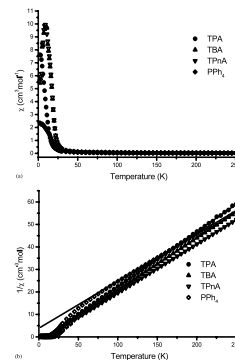


Simon G. Carling, Justin M. Bradley, Dirk Visser, Peter Day

Polyhedron 22 (2003) 2317

Magnetic and structural characterisation of the layered materials AMnFe(C₂S₂O₂)₃

A series of layered dithio-oxalate compounds have been studied by EXAFS, powder XRD and SQUID magnetometry.

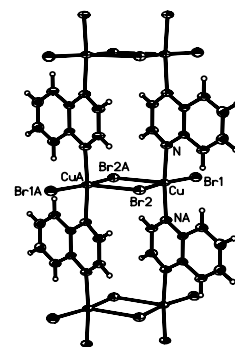


C.P. Landee, A. Delcheva, C. Galeriu, G. Pena, M.M. Turnbull, R.D. Willett

Polyhedron 22 (2003) 2325

Molecular-based quantum magnets: the isotropic spin ladder Cu(quinoxaline)Br₂

The structure, susceptibility, and high-field magnetization of μ -quinoxalinecopper(II) dibromide are reported. The compound crystallizes in the space group *C2/c* as a coordination polymer of neutral Cu₂Br₄ dimers bridged into chains by quinoxaline molecules forming a ladder structure.

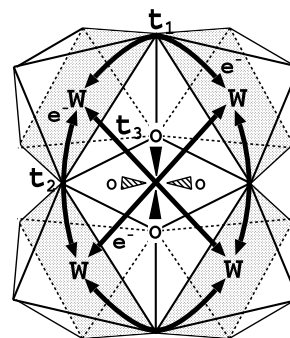


Nicolas Suaud, Alejandro Gaita-Ariño, Juan Modesto Clemente-Juan, José Sánchez-Marín, Eugenio Coronado

Polyhedron 22 (2003) 2331

Ab initio calculations of the transfer parameters and coulombic repulsion and estimation of their effects on the electron delocalization and magnetic coupling in mixed-valence Keggin polyoxotungstates

In this work, we present ab initio calculations on embedded fragments that permit to extract the value of the effective electron transfer integral and coulombic repulsion between W nearest neighbour atoms in a mixed-valence α PW₁₂O₄₀ Keggin polyoxoanion.

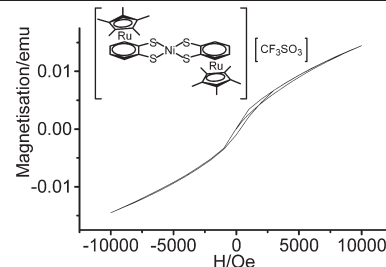


Neil Robertson, Satish Tiwary

Polyhedron 22 (2003) 2339

A new dithiolene complex magnet: $[\text{Ni}(\text{Cp}^*\text{Rubdt})_2][\text{CF}_3\text{SO}_3]$

The salt $[\text{Ni}(\text{Cp}^*\text{Rubdt})_2][\text{CF}_3\text{SO}_3]$ contains structural elements common to both metal-bis-1,2-dithiolene complexes and to metallocenes. Measurements of the temperature dependence of d.c. and a.c. magnetic susceptibility and magnetisation against field were consistent with bulk ferromagnetic order with a T_c of 3.5 K.

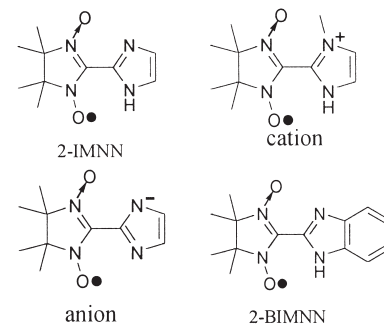


Tadashi Sugano, Stephen J. Blundell, William Hayes, Peter Day

Polyhedron 22 (2003) 2343

Magnetism in organic radical ion salts based on nitronyl nitroxide derivatives substituted with heterocyclic aromatic hydrocarbons

Magnetic properties of radical cation and anion salts of the neutral organic radicals, 2-imidazolyl and 2-benzimidazolyl nitronyl nitroxide (2-IMNN and 2-BIMNN) were investigated. The radical salts exhibit one-dimensional antiferromagnetic intermolecular interactions with the exchange coupling constants, which are significantly reduced from those observed in the neutral radicals, suggesting that the counter ions intercept intermolecular magnetic interactions.

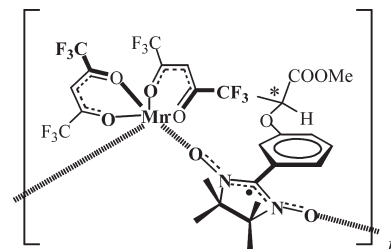


Maria Minguet, Dominique Luneau, Carley Paulsen, Elsa Lhotel, Alexander Gorski, Jacek Waluk, David B. Amabilino, Jaime Veciana

Polyhedron 22 (2003) 2349

From purely organic to metallo-organic chiral magnetic materials

There is presently a widespread search for materials which present magnetic ordering and appropriate chiroptical properties which would allow the observation of magneto-chiral effects. In this paper, we reflect on the possible uses of organic materials to probe this phenomenon, either as pure compounds or as their coordination compounds with metal ions.

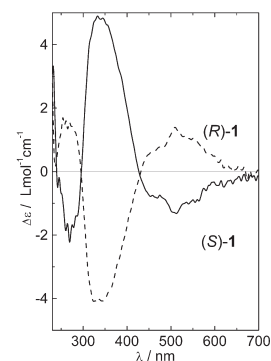


Neus Domingo, Philippe Gerbier, Jordi Gómez, Daniel Ruiz-Molina, David B. Amabilino, Javier Tejada, Jaime Veciana

Polyhedron 22 (2003) 2355

Synthesis and characterization of a new chiral nanomagnet

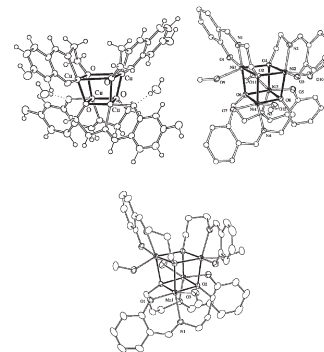
The dodecanuclear complexes formed between manganese ions and carboxylate anionic ligands are the single molecule magnets (SMMs) with greatest synthetic accessibility and richness of magnetic properties.



Masayuki Nihei, Norihisa Hoshino, Tasuku Ito, Hiroki Oshio*Polyhedron* 22 (2003) 2359

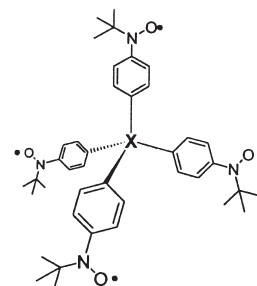
Structures and magnetic properties of metal cubes

Structures and magnetic properties of copper(II), nickel(II) and manganese(II) cubes are presented. In the cubes, four metal ions are assembled into the cubes by tridentate Schiff base ligands. Magnetic susceptibility measurements revealed the copper and nickel cubes have high-spin ground state, while the manganese cube has a $S = 0$ spin ground state.

**Martha Baskett, Paul M. Lahti, Fernando Palacio***Polyhedron* 22 (2003) 2363

Coordination complexes of a silicon-linked organic tetranitroxide

$\text{Mn}(\text{hfac})_2$ and $\text{Cu}(\text{hfac})_2$ form 1-D 1:1 coordination polymers with $\text{Si}(\text{O-TEMPO})_4$. Mn(II) exchange couples very strongly and antiferromagnetically within the TEMPO–Mn–TEMPO unit – even at room temperature – to give effectively $S = 3/2$ spin behavior. By comparison Cu(II) couples more weakly but ferromagnetically within TEMPO–Cu–TEMPO, with $J/k = (+)89$ K.

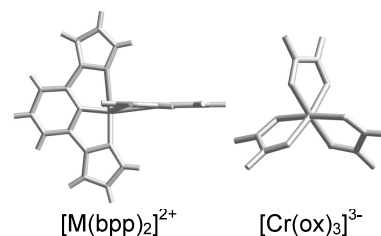


1 X = Si
2 X = C

Eugenio Coronado, Mari Carmen Giménez-López, Carlos Gimenez-Saiz, José M. Martínez-Agudo, Francisco M. Romero*Polyhedron* 22 (2003) 2375

Synthesis, structure and magnetic properties of iron (II), cobalt (II) and nickel (II) complexes of 2,6-bis(pyrazol-3-yl)pyridine (bpp) with $[\text{Cr}(\text{C}_2\text{O}_4)_3]^{3-}$ have been prepared. They were characterised by single-crystal X-ray diffraction, magnetic susceptibility measurements and thermal gravimetric analyses. All three compounds are isostructural and they are formed by isolated $[\text{M}^{\text{II}}(\text{bpp})_2]^{2+}$ and $[\text{Cr}(\text{C}_2\text{O}_4)_3]^{3-}$ complexes and free ClO_4^- .

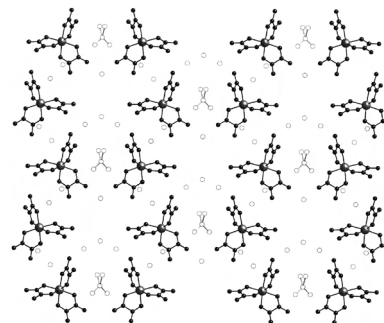
Iron (II), cobalt (II) and nickel (II) complexes of 2,6-bis(pyrazol-3-yl)pyridine (bpp) with $[\text{Cr}(\text{C}_2\text{O}_4)_3]^{3-}$ have been prepared. They were characterised by single-crystal X-ray diffraction, magnetic susceptibility measurements and thermal gravimetric analyses. All three compounds are isostructural and they are formed by isolated $[\text{M}^{\text{II}}(\text{bpp})_2]^{2+}$ and $[\text{Cr}(\text{C}_2\text{O}_4)_3]^{3-}$ complexes and free ClO_4^- .

**E. Coronado, J.R. Galán-Mascarós, C. Giménez-Saiz, C.J. Gómez-García, J.M. Martínez-Agudo, E. Martínez-Ferrero***Polyhedron* 22 (2003) 2381

Magnetic properties of hybrid molecular materials based on oxalato complexes

the radical salt of formula $\text{TTF}_3[\text{Ru}(\text{ox})_3] \cdot 0.5\text{EtOH} \cdot 4\text{H}_2\text{O}$ (1) which shows coexistence of paramagnetism and semiconducting properties. The second approach is the synthesis of extended 2D bimetallic oxalato-bridged networks of general formula $[\text{FeCp}_2^*][\text{M}^{\text{II}}\text{Rh}(\text{ox})_3]$ in which paramagnetic layers of decamethylferricinium cations are alternated with paramagnetic bimetallic layers.

The use of $[\text{M}^{\text{III}}(\text{ox})_3]^{3-}$ ($\text{M}^{\text{III}} = \text{Ru}, \text{Rh}$) complexes as building blocks for hybrid molecular materials is highlighted with two different synthetic approaches. The first strategy is the combination of organic donors and $[\text{Ru}^{\text{III}}(\text{ox})_3]^{3-}$ units, resulting in

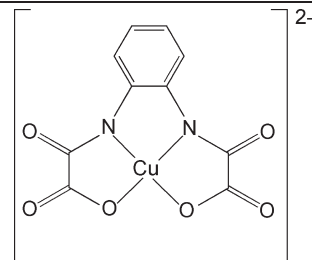


C.L.M. Pereira, E.F. Pedroso, M.A. Novak,
A.L. Brandl, M. Knobel, H.O. Stumpf

Polyhedron 22 (2003) 2387

Cluster glass-like behavior in a 2D bimetallic
molecule-based magnet

The reaction of the $\text{Na}_2\text{Cu}(\text{opba})$ building block with the $\text{Co}(\text{II})$ ion leads to the molecule-based magnet formula of $\text{Na}_2[\text{Co}_2\{\text{Cu}(\text{opba})\}_3] \cdot 2\text{DMSO} \cdot 6\text{H}_2\text{O}$ where *opba* stands for *ortho*-phenylenebis(oxamato). Magnetic properties have been investigated in the 2–300 K temperature range. The compound presents a large coercive field, around 3.5 kOe, and the AC susceptibility measurements have revealed a cluster glass-like behavior.

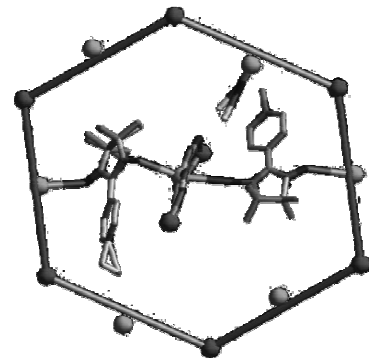


M.A. Novak, M.G.F. Vaz, N.L. Speziali,
W.V. Costa, H.O. Stumpf

Polyhedron 22 (2003) 2391

Magnetic properties of an interlocked molecular magnet

In this work we report the magnetic properties and preliminary structural results of the molecule-based ferrimagnet with formula $[\text{Pr-Rad}]_2[\text{Mn}_2\{\text{Cu}(\text{opba})\}_3](\text{DMSO})_{3.3} \cdot 5\text{H}_2\text{O}$, where *opba* stands for *ortho*-phenylenebis(oxamato) and Pr-Rad^+ is propyl-nitronyl nitroxide radical cation, which presents magnetic transition at 24.1 K.

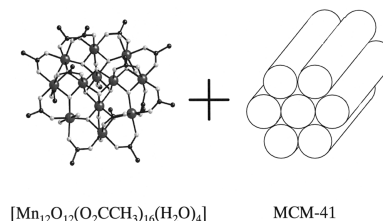


M. Clemente-León, E. Coronado, A.
Forment-Aliaga, J.M. Martínez-Agudo, P.
Amorós

Polyhedron 22 (2003) 2395

Mn_{12} single-molecule magnets incorporated
into mesoporous MCM-41 silica

The incorporation of four Mn_{12} derivatives, namely $[\text{Mn}_{12}\text{O}_{12}(\text{O}_2\text{CR})_{16}(\text{H}_2\text{O})_4]$ ($\text{R} = \text{CH}_3$ (1), CH_3CH_2 (2), C_6H_5 (3), C_6F_5 (4)), into the hexagonal channels of the MCM-41 mesoporous silica have been studied. Only the smallest clusters 1 and 2 that are those with compatible size with the pores of MCM-41 could be incorporated into the mesoporous silica. Powder X-ray diffraction (XRD) analysis and N_2 adsorption–desorption isotherm experiments show that the well-ordered hexagonal structure of MCM-41 is preserved and that the Mn_{12} clusters are inside the pores.

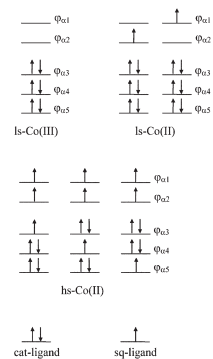


Sophia I. Klokishner, O.S. Reu

Polyhedron 22 (2003) 2401

Vibronic dynamic problem of valence tautomerism in cobalt compounds. Magnetic and optical properties

The model employed takes into account the main physical factors responsible for the temperature transformations of optical spectra and magnetic properties: intramolecular transfer of the excess electron, vibronic and exchange interactions. For a single valence tautomeric complex the vibronic problem of pseudo-Jahn-Teller effect is solved. The suggested model is in qualitative agreement with the experimental data.

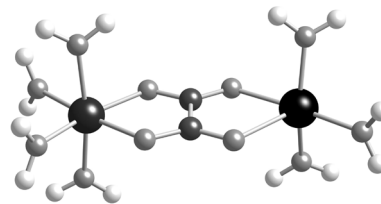


David Taratiel, Jesús Cabrero, Coen de Graaf, Rosa Caballol

Polyhedron 22 (2003) 2409

Magnetic coupling in oxalato-bridged hetero-bimetallic compounds: an ab initio study

Multiconfigurational perturbation theory (CASPT2) and difference dedicated configuration interaction are applied to study the ferromagnetic coupling in model oxalato-bridged Cr(III)Cu(II) and Cr(III)Ni(II) molecular species. The experimental coupling is very well reproduced at both calculation levels when the model nearly reproduces the experimental geometrical structure.

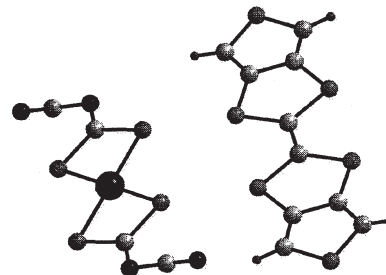


Xavi Ribas, Marta Mas-Torrent, Concepció Rovira, Jaume Veciana, João C. Dias, Helena Alves, Elsa B. Lopes, Manuel Almeida, Klaus Wurst

Polyhedron 22 (2003) 2415

Molecular compounds based on DT-TTF and Au(cdc)₂ complex. Structural, magnetic and electrical properties

The synthesis and characterisation of two new radical ion salts based on the donor dithiophenetetrathiafulvalene (DT-TTF) and the anion Au(cdc)₂⁻ (cdc = cyanodithioimido carbonate) are described. These salts were characterised as the mixed valence compound (DT-TTF)₂(Au(cdc)₂) (1) and the completely ionic salt (DT-TTF)(Au(cdc)₂) (2). The X-ray crystal structure of both compounds was determined. The electrical conductivity was measured in a single crystal at room temperature magnetic measurements were performed.

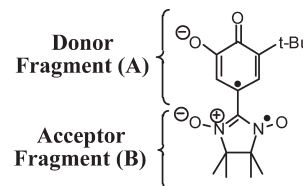


David A. Shultz

Polyhedron 22 (2003) 2423

The donor-acceptor contributions to ferromagnetic exchange coupling in heterospin biradicals

Frontier orbital analysis provides insight into a donor-acceptor contribution to ferromagnetic exchange in biradicals having two, chemically distinct paramagnetic groups. Heterospin species might have inherently stronger ferromagnetic coupling than homospin biradicals. Thus, considering ferromagnetic exchange coupling from a donor-acceptor perspective embodies an important structure-property relationship for designing high-spin molecules.

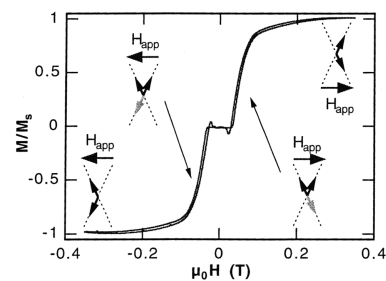


Raluca Tiron, Wolfgang Wernsdorfer, Fabien Tuyeras, Ariane Sculler, Valérie Marvaud, Michel Verdaguer

Polyhedron 22 (2003) 2427

Hexacyanometalate molecular chemistry: trinuclear CrNi₂ complexes; micro-SQUID magnetisation studies of intermolecular interactions

The magnetisation of the three trinuclear CrNi₂ complexes (*S* = 7/2 ground spin state) is studied on single crystals, using micro-SQUID technique. The complex and apparently strange magnetisation behaviour in the magnetically ordered phase (graphics) is readily interpreted by canted ferromagnetic interaction between molecules having two different orientations in the crystal.

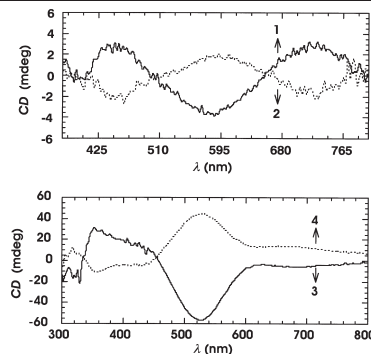


**E. Coronado, C. Giménez-Saiz,
J.M. Martínez-Agudo, A. Nuez,
F.M. Romero, H. Stoeckli-Evans**

Polyhedron 22 (2003) 2435

Design of chiral magnets: cyanide-bridged bimetallic assemblies based on cyclohexane-1,2-diamine

Four magnetic compounds based on chiral ligands *trans*-(1*S*,2*S*)-chxn and *trans*-(1*R*,2*R*)-chxn (chxn: cyclohexane-1,2-diamine), $[\text{Ni}(\textit{trans}\text{-}(1*S*,2*S*\text{-chxn})_2)_3[\text{Fe}(\text{CN})_6]_2 \cdot 2\text{H}_2\text{O}$ (**1**), $[\text{Ni}(\textit{trans}\text{-}(1*R*,2*R*\text{-chxn})_2)_3[\text{Fe}(\text{CN})_6]_2 \cdot 2\text{H}_2\text{O}$ (**2**), $[\text{Cu}(\textit{trans}\text{-}(1*S*,2*S*\text{-chxn})_2)_3[\text{Fe}(\text{CN})_6]_2 \cdot 4.5\text{H}_2\text{O}$ (**3**) and $[\text{Cu}(\textit{trans}\text{-}(1*R*,2*R*\text{-chxn})_2)_3[\text{Fe}(\text{CN})_6]_2 \cdot 4.5\text{H}_2\text{O}$ (**4**), are reported. The four compounds are chiral, as confirmed by X-ray analyses and circular dichroism measurements. From the magnetic point of view, **1** and **2** behave as ferromagnets, whereas **3** and **4** show a paramagnetic behavior.

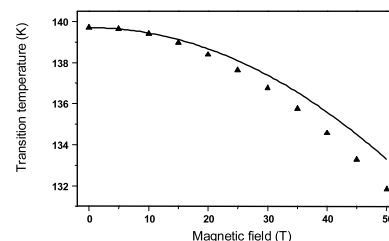


Christophe Conséjo, Gábor Molnár, Michel Goiran, Azzedine Bousseksou

Polyhedron 22 (2003) 2441

Two-level Ising-like model for spin-crossover phenomenon including the magnetic field effect: the mean-field approximation and Monte Carlo resolutions

In this paper we analysed the magnetic field effect on the spin-crossover phenomenon using different theoretical approaches: thermodynamic and Ising-like models.

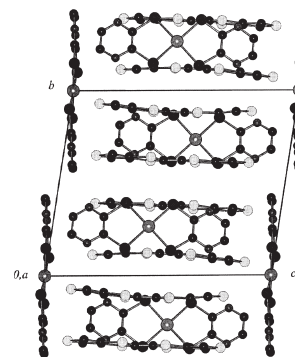


João C. Dias, Jorge Morgado, Helena Alves, Elsa B. Lopes, Isabel C. Santos, M.T. Duarte, R.T. Henriques, Manuel Almeida, Xavier Ribas, Concepción Rovira, Jaume Veciana

Polyhedron 22 (2003) 2447

Magnetic and electrical properties of $(\text{DT-TTF})_4[\text{Au}(\text{pds})_2]_3$

The charge transfer salt $(\text{DT-TTF})_4[\text{Au}(\text{pds})_2]_3$ (DT-TTF, $\Delta^{2,2'}$ -bithieno[3,4-d]-1,3-dithiol; pds, pyrazine-2,3-diselenate) was prepared and characterised by X-ray diffraction, electrical conductivity, thermoelectric power, magnetic susceptibility and EPR measurements. This compound crystallises in the triclinic system, space group $P\bar{1}$, with the unit cell parameters $a = 9.712(5)$ Å, $b = 13.620(5)$ Å, $c = 17.169(5)$ Å, $\alpha = 97.254(5)^\circ$, $\beta = 106.132(5)^\circ$, $\gamma = 95.956(5)^\circ$, $V = 2141.10(15)$ Å³, $Z = 1$.



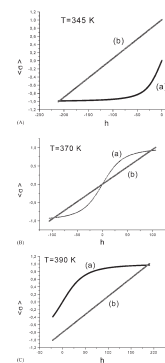
Jorge Linares, Cristian Enachescu, Kamel Boukheddaden, François Varret

Polyhedron 22 (2003) 2453

Monte Carlo entropic sampling applied to spin crossover solids: the squareness of the thermal hysteresis loop

The Monte Carlo entropic sampling method previously presented is adapted here to an Ising-like system with short- and long-range interactions. Such model is suited to spin crossover solids where the long interaction is due to elastic coupling mediated by the

lattice, while the short-range interaction originates from the bonding between the spin crossover units. The numerical method has been tested successfully by comparison to the exact solution for a 1D system. We describe here the results obtained for 2D systems, and show that the squareness of the thermal hysteresis loop, associated with the spin-transition, can be correlated to the strength of short-range interactions.

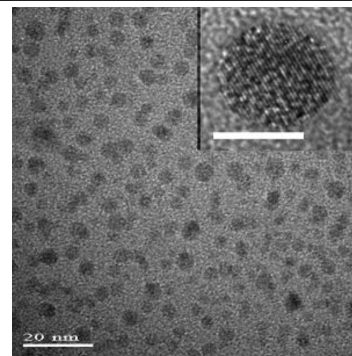


Ian Gilbert, Angel Millán, Fernando Palacio, Andrea Falqui, Etienne Snoeck, Virginie Serin

Polyhedron 22 (2003) 2457

Magnetic properties of maghemite nanoparticles in a polyvinylpyridine matrix

Magnetic measurements have been carried out on nanocomposites consisting of individual maghemite ($\gamma\text{-Fe}_2\text{O}_3$) particles distributed throughout a polyvinylpyridine matrix with a range of particle sizes and concentrations. Magnetic measurements and particle size measurements have been compared to investigate particle size effects upon magnetic properties.

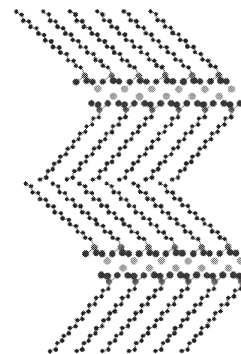


Elvira M. Bauer, Carlo Bellitto, Said A. Ibrahim, Mohamed R. Mahmoud, Guido Righini

Polyhedron 22 (2003) 2463

Ni(II)octadecylphosphonate: an inorganic/organic layered weak-ferromagnet

$\text{Ni}[\text{CH}_3(\text{CH}_2)_{17}\text{PO}_3]\cdot\text{H}_2\text{O}$ was obtained from $\text{NiCl}_2\cdot 6\text{H}_2\text{O}$ and the octadecylphosphonic acid in water. It crystallises in the orthorhombic space group $Pmn2_1$. The crystal lattice consists of alternating inorganic and organic layers: the former made of octahedral $[\text{NiO}_6]$ chromophores the latter of bi-layers of octadecylphosphonate ligands. It represents an interesting example of a weak-ferromagnetic insulator.

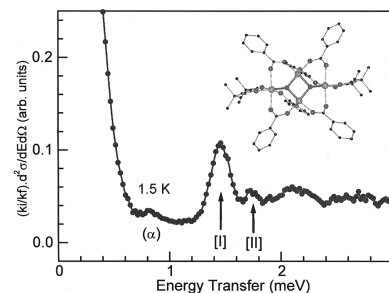


R. Basler, G. Chaboussant, C. Cañada-Vilalta, G. Christou, H. Mutka, S. Janssen, F. Altorfer, H.-U. Güdel

Polyhedron 22 (2003) 2471

Magnetic and inelastic neutron scattering studies of a frustrated tetranuclear Mn^{3+} butterfly-type cluster

INS spectra at $\lambda = 4.3 \text{ \AA}$ and 1.5 K of the tetra-nuclear Mn(II) complex $[\text{Mn}_4\text{O}_2(\text{O}_2\text{-CPh})_6(\text{dpm})_2]$. Along with bulk magnetic measurements, magnetic peaks (I) and (II) shown in this figure enabled the determination of the single-ion anisotropy terms as well as the exchange interactions within the cluster.

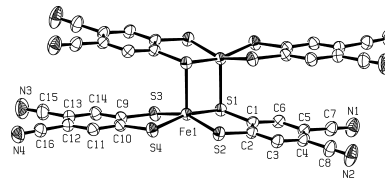


H. Alves, D. Simão, H. Novais, I.C. Santos, C. Giménez-Saiz, V. Gama, J.C. Waerenborgh, R.T. Henriques, M. Almeida

Polyhedron 22 (2003) 2481

$(n\text{-Bu}_4\text{N})_2[\text{Fe}(\text{dcbdt})_2]_2$. Synthesis, crystal structure and magnetic characterisation

The $(n\text{-Bu}_4\text{N})_2[\text{Fe}(\text{dcbdt})_2]_2$ complex, where dcbdt = 4,5-dicyanobenzene-1,2-dithiolate, was prepared and characterised by X-ray diffraction, Mössbauer spectroscopy and magnetisation measurements. The magnetic susceptibility shows that the dimerised $[\text{Fe}(\text{dcbdt})_2]$ -units have a low spin $S = 1/2$ configuration.

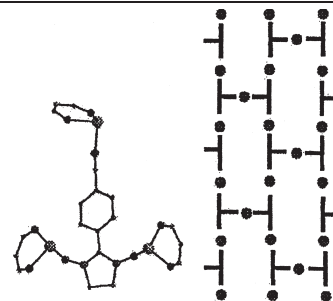


O.V. Koreneva, G.V. Romanenko, Yu. G. Shvedenkov, V.N. Ikorskii, V.I. Ovcharenko

Polyhedron 22 (2003) 2487

Molecular magnets based on $M(\text{hfac})_2$ and spin-labeled nitrite

New types of $\text{Cu}(\text{hfac})_2\text{L}$ chain polymorphs and new examples of layered molecular magnets ordering at 9.1 ($[\text{Mn}(\text{hfac})_2]_3\text{L}_2$) and 11.9 K ($[\text{Co}(\text{hfac})_2]_3\text{L}_2$) are described.

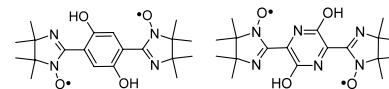


Eugene V. Tretyakov, Ilia V. Eltsov, Sergey V. Fokin, Yurii G. Shvedenkov, Galina V. Romanenko, Victor I. Ovcharenko

Polyhedron 22 (2003) 2499

Synthesis of 2-iminonitroxide-substituted phenols and pyridine-3-oles. Copper(II) complexes with imino nitroxides containing 2-hydroxyphenyl substituents

Methods for the synthesis of a new family of nitronitroxides, iminonitroxides, and their precursors with 2-hydroxyphenyl or 3-hydroxypyridin-2-yl substituents in the side chain have been developed. Five heterospin chelates of Cu(II) with deprotonated iminonitroxides have been isolated. Their structure and magnetic properties have been studied.

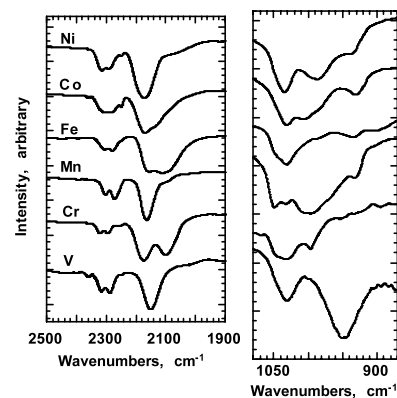


Shireen R. Marshall, Jesper Bendix, Aphichart Rodchanarowan, Joel S. Miller

Polyhedron 22 (2003) 2515

Synthesis, characterization, and magnetic properties of tetracyanonitridochromates

The reaction of $S = 1/2$ $[\text{PPh}_4]_2[\text{Cr}^{\text{V}}(\text{N}(\text{CN})_4)]$ with $[\text{M}(\text{NCMe})_x][\text{BF}_4]_2$ ($M = \text{V}, \text{Fe}, \text{Co}, \text{Ni}, x = 6; M = \text{Mn}, x = 4$) and $[\text{Cr}^{\text{II}}(\text{NCMe})_6](\text{BARF})_2$ [BARF = tetrakis(3,5-trifluoromethylphenyl)borate] led to materials of nominal $\text{M}^{\text{II}}[\text{Cr}^{\text{V}}(\text{N}(\text{CN})_4)] \cdot \text{MeCN}$ composition, albeit contaminated with cationic and/or anionic impurities.

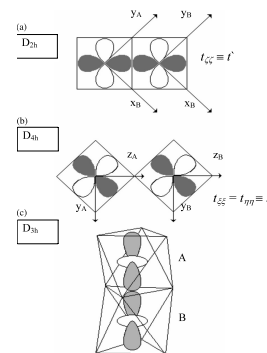


J.J. Borrás-Almenar, E. Coronado, J.M. Clemente-Juan, A.V. Pali, B.S. Tsukerblat

Polyhedron 22 (2003) 2521

Problem of the magnetic anisotropy in orbitally degenerate exchange and mixed-valence clusters

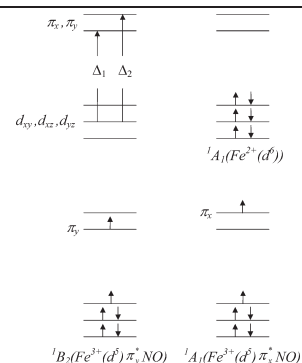
This contribution summarizes the results obtained in the problem of orbital degeneracy of the metal ions in exchange coupled and mixed-valence (MV) clusters.



E. Coronado, S. Klokishner, O. Reu, B. Tsukerblat
Polyhedron 22 (2003) 2527

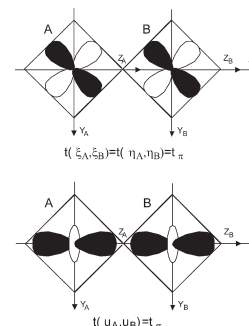
A pseudo-Jahn–Teller model of the photochromic effect in sodium nitroprusside

A new model for the photochromic effect in sodium nitroprusside $\text{Na}_2[\text{Fe}(\text{CN})_5(\text{NO})] \cdot 2\text{H}_2\text{O}$ based on the concept of the pseudo-Jahn–Teller effect is proposed. The model takes into account the electron transfer from the Fe^{2+} ion to the π^* orbitals of the NO-ligand as well as the vibronic mixing of three electronic states of the Fe–NO fragment through the non-symmetric and full-symmetric modes. The problem is solved within the adiabatic approximation.


Andrei V. Pali, Boris S. Tsukerblat, Eugenio Coronado, Juan M. Clemente-Juan, Juan J. Borrás-Almenar
Polyhedron 22 (2003) 2537

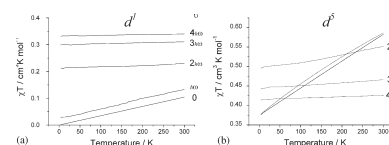
Orbitally dependent kinetic exchange in cobalt(II) pairs: origin of the magnetic anisotropy

A comprehensive theoretical study of the magnetic exchange between Co^{2+} ions is reported. We elucidate the major electronic factors controlling the exchange anisotropy in the Co(II) pairs. The degree of the magnetic anisotropy is shown to depend on the strength of the cubic crystal field and on the relative efficiency of electron transfer pathways contributing to the kinetic exchange. An unusual role of spin–orbit interaction is revealed. This interaction tends to reduce the anisotropy caused by the orbitally dependent exchange. Finally, we discuss conditions of the applicability of the conventional isotropic Lines' model.


Kim R. Dunbar, Eric J. Schelter, Boris S. Tsukerblat, Sergei M. Ostrovsky, Vadim Yu. Mirovitsky, Andrew V. Pali
Polyhedron 22 (2003) 2545

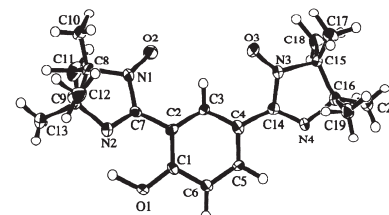
Magnetic properties of complex d^1 and d^5 ions: crystal field model and Jahn–Teller effect

The magnetic behavior, including anisotropic g -values and temperature dependent magnetic susceptibility, has been calculated for d^1 and d^5 ions possessing 2T_2 ground states. The model accounts for spin–orbit coupling, an axial (trigonal or tetragonal) crystal field, and, in the framework of the semi-classic adiabatic approximation, vibronic Jahn–Teller and pseudo Jahn–Teller interactions acting within the ground manifold.


Takayuki Ichimura, Kentaro Doi, Chiemi Mitsuhashi, Takayuki Ishida, Takashi Nogami
Polyhedron 22 (2003) 2557

meta-Phenylene-bridged bis(imino nitroxide) biradicals as potential high-spin ligands

Frozen-solution ESR spectra of 4-hydroxy-1,3-phenylenebis(imino nitroxide) (**1**) suggest that **1** has a ground triplet state. The magnetic measurements of $\text{Cu}(\text{L}^1)_2$, where L^1 is the anionic form derived from **1**, indicated the presence of ferromagnetic interaction ascribable to directly bonded copper(II)–radical moieties.



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